

Cohesive Particle Model using the Discrete Element Method on the Yade platform

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Outline

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particle
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Particle models history

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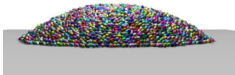
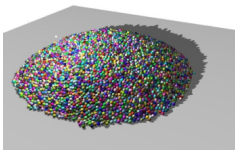
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- in mechanics since 1970 (Cundall, soil mechanics)
- continuum=particles+contacts, relatively simple contact laws
- suitable for “discontinua” behavior
- different flavors of particle methods (DOF number, static/dynamic problem, particle type)

Classification

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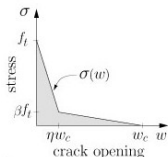
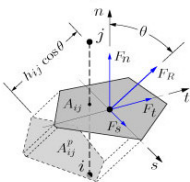
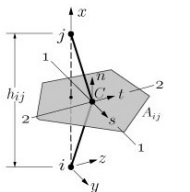
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- lattice models (no mass, 3/6 DOFs, spring/beam links between particles; 2D variants)
- mass-spring (3 DOFs, explicit dynamics)
- DEM (discrete element method) — particles with 6 DOFs, rigid shape (rigid), inter-particle collisions
- DEM+FEM (“multi-body dynamics”) — particles are deformable (FEM) and collide (DEM)

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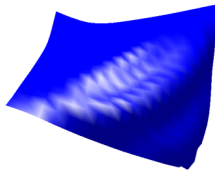
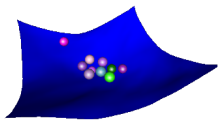
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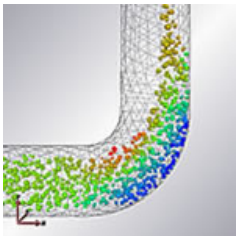
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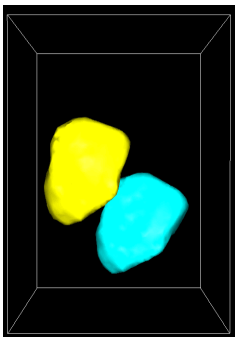
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DEM and DEMs

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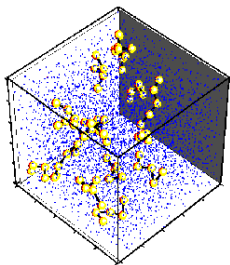
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■ smooth

- collision prediction
- t – between collisions
- restitution equations
- gas dynamics (few contacts)

■ non-smooth

- collision as shape overlaps
- t – a given Δt
- repulsive force, integration of motion equations
- dense packings

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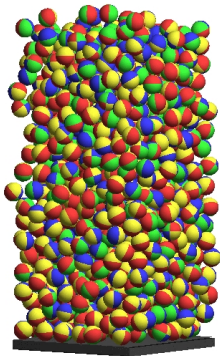
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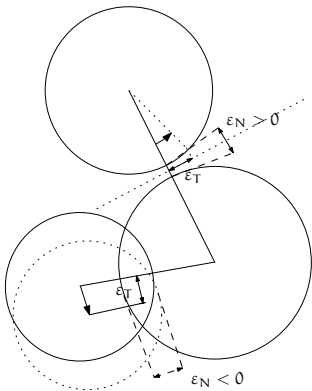
- concrete (generally cohesive-frictional materials)
- contacts have 3 DOFs: normal and shear strains ϵ_N, ϵ_T and stresses σ_N, σ_T
- model features:
 - tensile damage + visco-damage
 - compressive plasticity
 - shear plasticity + visco-plasticity
- parameters mostly with a physical meaning
- calibration procedures designed

Normal stress evaluation

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$$\sigma_N = [1 - \omega H(\varepsilon_N)] k_N \varepsilon_N + \sigma_{Nv}(\dot{\varepsilon}_{Nd})$$



ε_N normal strain

k_N contact normal modulus

ω internal damage variable,
 $\omega = g(\kappa)$, $\kappa = \max \varepsilon_N$

$g(\kappa)$ damage evolution function
(parameters ε_0 and ε_f)

σ_{Nv} damage overstress,
evaluated iteratively from
induced damage strain rate
 $\dot{\varepsilon}_{Nd}$ (τ_d , M_d)

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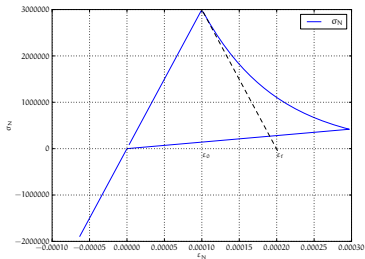
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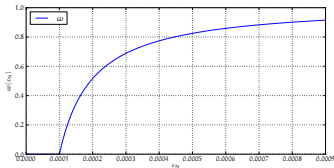
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$$\omega = g(\kappa) = 1 - \frac{\varepsilon_f}{\kappa} \exp\left(-\frac{\kappa - \varepsilon_0}{\varepsilon_f}\right)$$

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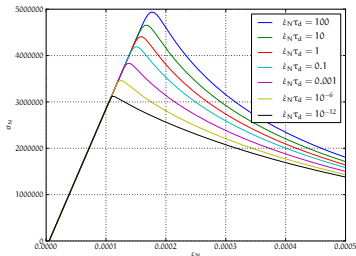
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$$\sigma_{Nv}(\dot{\varepsilon}_{Nd}) = k_N \varepsilon_0 \langle \tau_d \dot{\varepsilon}_{Nd} \rangle^{M_d}$$

Shear stress evaluation (after σ_N)

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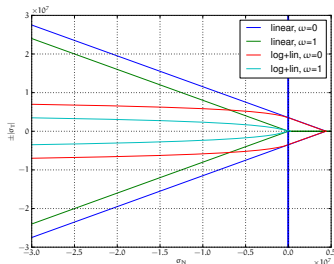
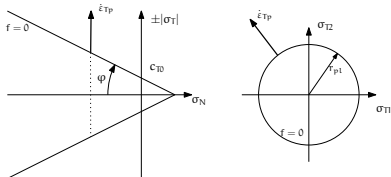
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Shear stress, plasticity function, plastic flow rule

$$\sigma_T = k_T(\epsilon_T - \epsilon_{Tp})$$

$$f(\sigma_N, \sigma_T) = |\sigma_T| - (c_{T0}(1 - \omega) - \sigma_N \tan \varphi)$$

$$\dot{\epsilon}_{Tp} = \dot{\lambda} \frac{\sigma_T}{|\sigma_T|}$$



Model parameters

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Elastic parameters

moduli k_N , k_T , interaction radius R_I .

Plasticity+damage parameters

limit elastic strain ε_0 , damage evolution parameter ε_f ; friction angle φ , cohesion c_{T0} .

Viscosity parameters

characteristic time τ_d , exponent M_d ; (τ_{pt} , M_{pt})

Confinement parameters

hardening strain ε_s , hardening modulus \tilde{K}_s , plasticity function parameter Y_0 .

Calibrable properties

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Scalar values

- Young's modulus E , Poisson's ratio ν
- tensile and compressive strengths f_t , f_c ,
- fracture energy G_f .

Qualitative matching

- confinement behavior
- rate-dependent behavior

Uniaxial tension and compression

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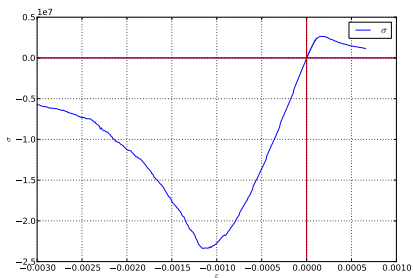
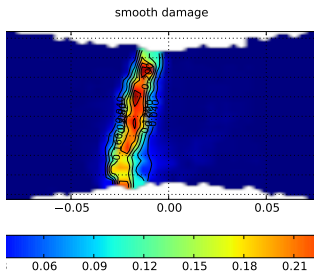
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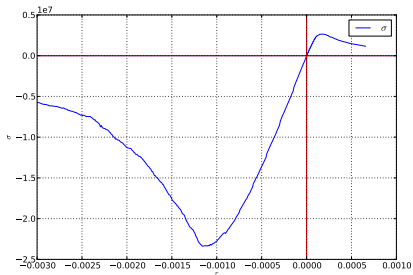
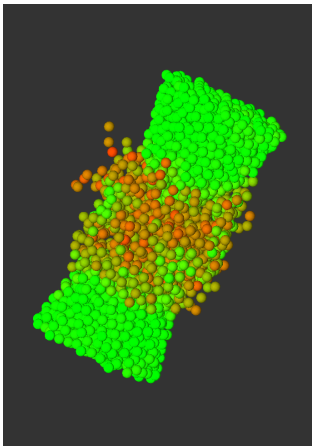
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Bending setup

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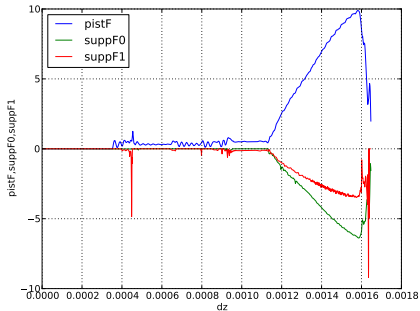
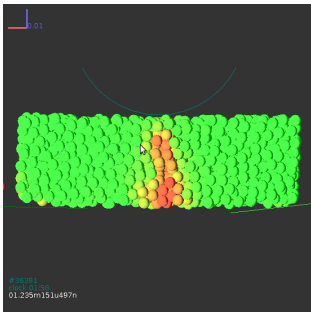
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Confined compression

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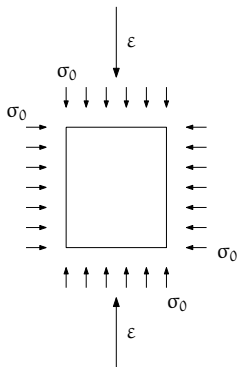
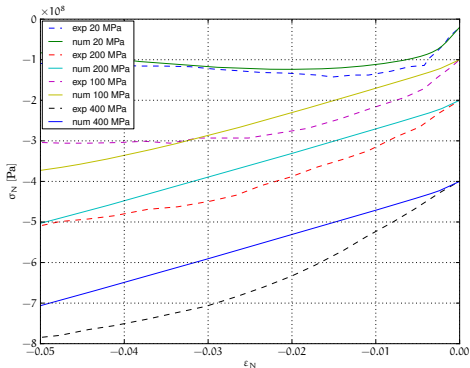
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Tensile rate effect

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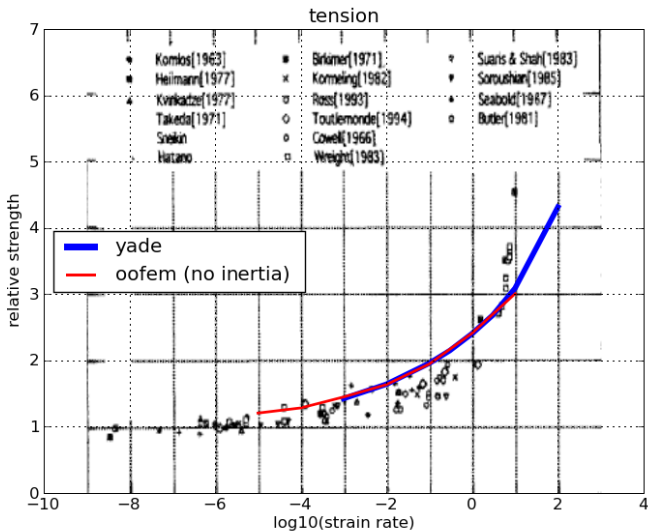
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Compressive rate effect

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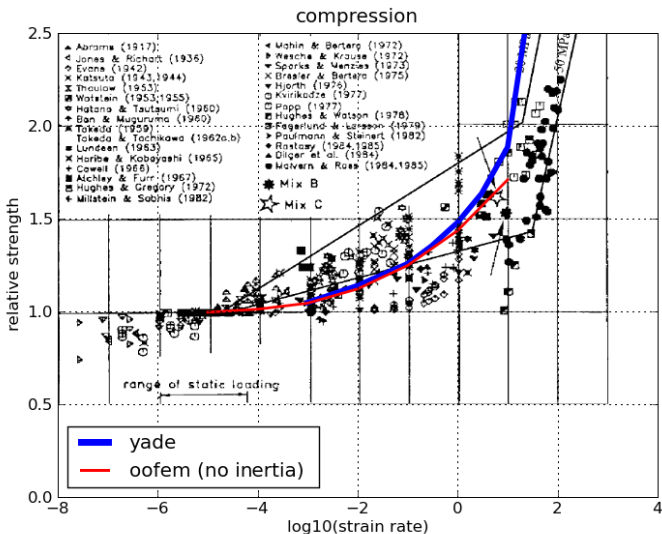
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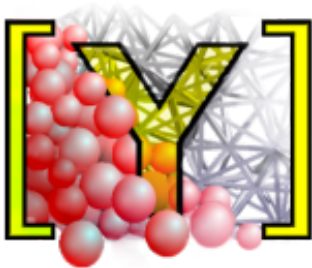
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www.yade-dem.org
launchpad.net/yade

- initiated 2004 by Frédéric Donzé
- in c++, on Linux/Unix
- object-oriented, “toolkit of algorithms”
- substantially reworked during the thesis
 - documentation
 - parallel computation
 - batch scheduling system
 - profiling, debugging tools
 - python interface 🐍

Python as the interface

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- scripting language, large library, similar to matlab
- easy to interface with fortran/c/c++
- Yade classes mirrored in python
- scripts efficient for simulation setup, postprocessing
- compatible over Yade's internal changes
- runtime control & debugging from the command line

Data components

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Body (particle)

Shape Sphere, Facet, ...

Material ElastMat, FrictMat, ...

State position, orientation, velocity, ...

Bound for approximate collision detection (**Aabb**)

Generalized forces

Interaction of 2 bodies

InteractionGeometry different for **Sphere+Sphere**,
Facet+Sphere, ...

InteractionPhysics internal state of interaction (plasticity
variables, damage, history)



Functional components

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Engines

- **GlobalEngine** act on all bodies/interactions
- **PartialEngine** act on some bodies/interactions
- **Dispatcher** calls functions based on classes of arguments:
e.g. **Facet+Sphere** needs different function than
Sphere+Sphere collision

Functors

Callable function-like objects. Accept only certain classes and are called by **Dispatchers**.

Simulation structure

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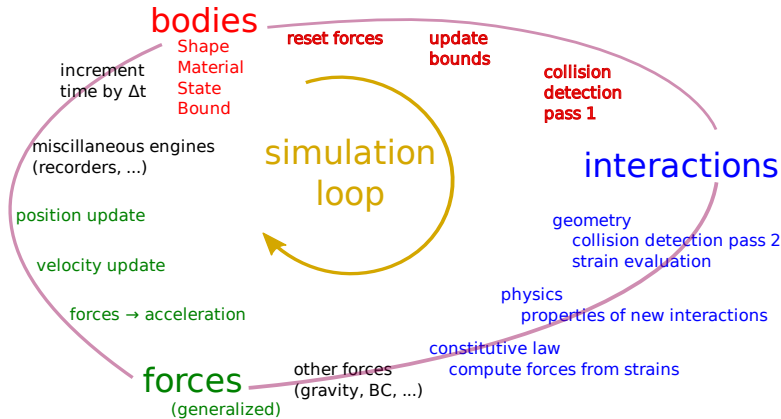
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What it looks like in python I.

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Simulation loop in code

```
O.engines=[  
    ForceResetter(),  
    BoundDispatcher([Bo1_Sphere_Aabb(),Bo1_Facet_Aabb()]),  
    InsertionSortCollider(),  
    InteractionDispatchers(  
        [lg2_Sphere_Sphere_Dem3DofGeom(), lg2_Facet_Sphere_Dem3DofGeo  
        [lp2_FrictMat_FrictMat_FrictPhys()],  
        [Law2_Dem3Dof_FrictPhys_Basic()],  
    ),  
    GravityEngine(gravity=(0,0,-9.81)),  
    NewtonIntegrator()  
]
```

lg2 2-ary functor creating **InteractionGeometry** (Bo1, lg2, lp2, Law2)

Facet_Sphere accepting **Facet** and **Sphere** as its arguments

Dem3DofGeom returning **Dem3DofGeom** instance

What it looks like in python II.

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Simulation data in code

```
O.materials.append(  
    FrictMat(young=30e9,poisson=.3,density=3000,frictionAngle=.5)  
)  
O.bodies.append([  
    utils.sphere((0,0,3),radius=1),  
    utils.facet([(-1,-1,0),(1,0,0),(0,1,0)])  
])  
O.dt=.5*utils.PWaveTimeStep()
```

Running simulation

```
O.run(10000); O.wait()    # Basic simulation control  
O.save('/tmp/a.xml')  
print O.bodies[3].state.vel    # inspection of (c++) data  
print O.interactions[0,2].geom.normal  
print O.materials[0].young  
quit()
```


Engines

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Loading control (BoundaryControllers)

TriaxialStressController (stress/strain rate),
UniaxialStrainer (strain control), **PerilsoCompressor**
(periodic iso-stress), **Peri3dController** (periodic stress tensor)

Applying conditions

GravityEngine (constant gravity field), **ForceEngine**,
RotationEngine, **TranslationEngine**, ...

Algorithms

InsertionSortCollider (collision detection), **NewtonIntegrator**
(2nd order central-differences explicit integration scheme),
GlobalStiffnessTimeStepper (adjust timestep based on
packing stiffness)

Particles and interactions

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Shapes

Sphere, Facet, Wall, Box. (Tetra, polyhedral grains, ...).

Handling collisions (InteractionGeometry)

Handling collisions of $2 \times$ **Sphere, Facet+Sphere, Box+Sphere, Wall+Sphere.**

Constitutive laws

Dry friction (classical DEM), **Mindlin's contact**, **Plassiard's formulation**, **Cohesive-frictional model**, **rock model**, **concrete model**, **capillary effects** between grains. (more outside source tree or undocumented)

Coupling

OpenFOAM, Comsol, fluids.



Outline

Cohesive
particle
model &
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Václav
Šmilauer

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Jan Kozicki, Grenoble

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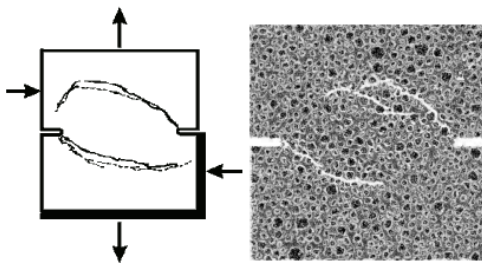
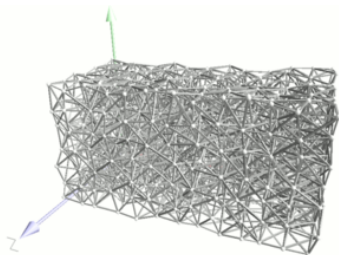
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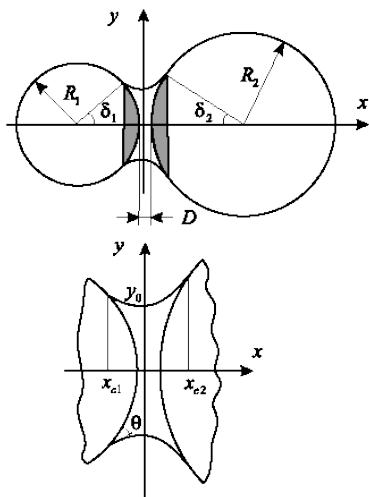
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3d lattice model of
tensile concrete
fracture.



Behavior of
granular media
with capillary
effects between
grains.

Wenjie Shiu, Grenoble

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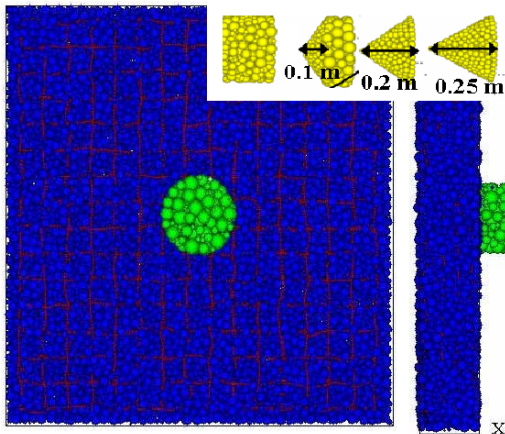
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Missile impact on
concrete
structures.

Wenjie Shiu, Grenoble

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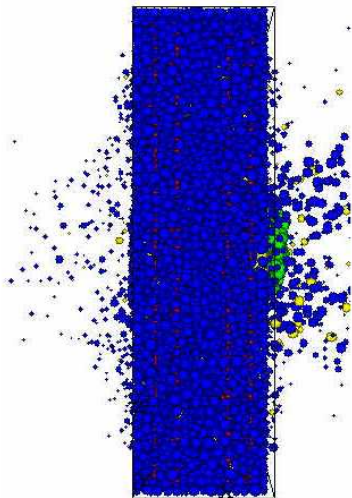
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structures.

Emanuele Catalano, Grenoble

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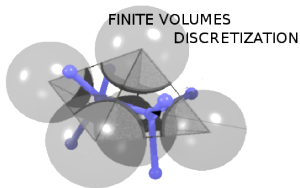
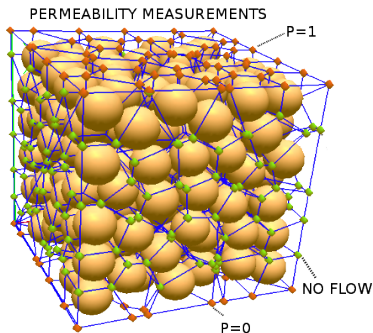
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A finite
volumes-DEM
coupled
formulation for
fluid-solid
interactions in
granular media.

Benoît Charlas, Grenoble

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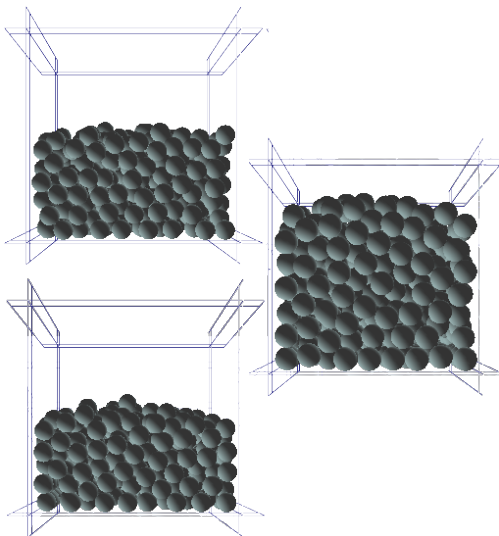
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Hydride metal
powders in
hydrogen storage
tanks — swelling
& shrinking due to
chemical reactions
with hydrogen,
creating
mechanical effects.

Sergei Dorofeenko, Moscow

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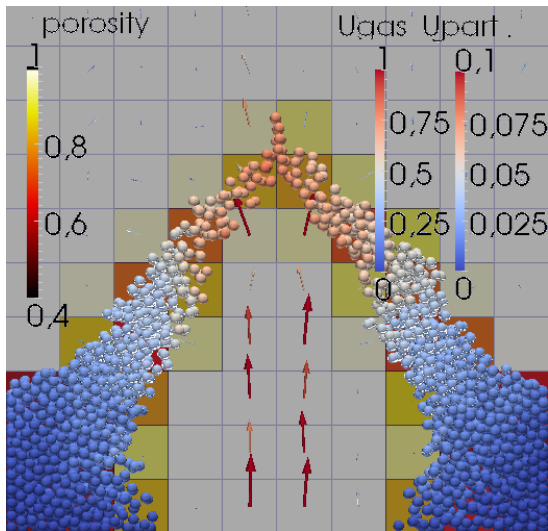
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Coupling
Computational
Flow Dynamics
(CFD) and DEM
— OpenFOAM
and Yade.

Anton Gladky, Freiberg

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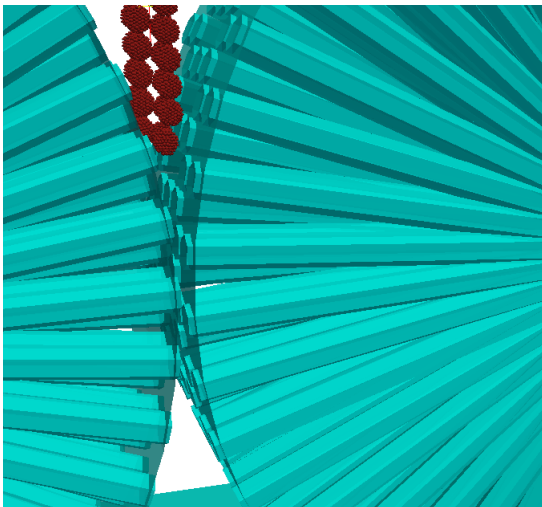
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Mineral processing
— analyzing rock
destruction in the
machine.

Anton Gladky, Freiberg

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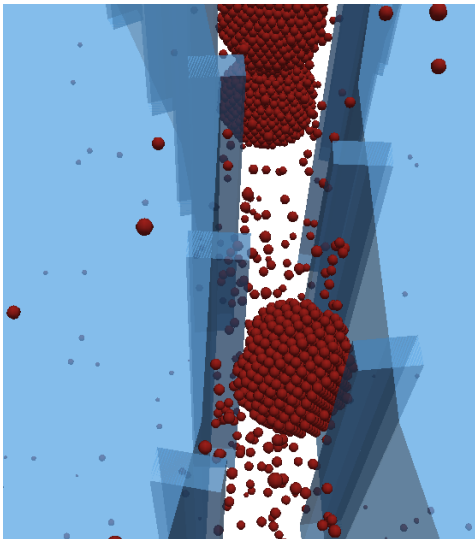
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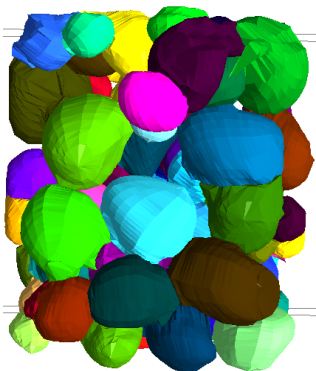
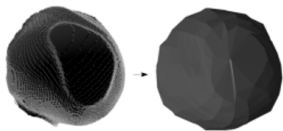


Mineral processing
— analyzing rock
destruction in the
machine.

Alsidqi Hasan, Grenoble

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Modeling snow
grains based on
CT scans, as
polyhedra which
can deform along
crystallographic
planes.

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Franck Lominé, Nantes

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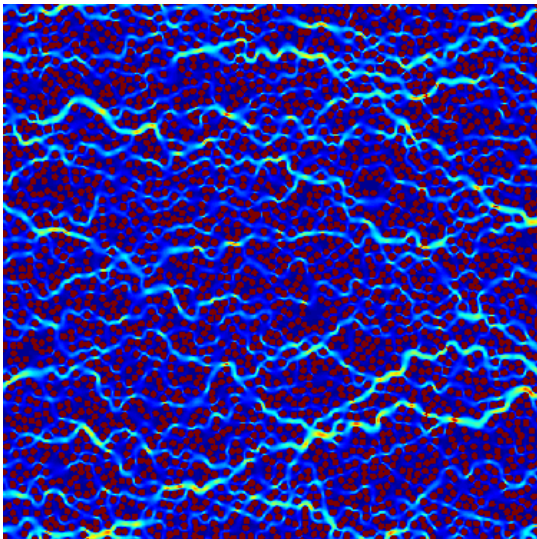
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Interaction
between
DEM-modeled
solid and Lattice
Boltzmann
Method (LBM)
modeled fluid.
(Started by Luc
Scholtès)

Chiara Modenese + Boon Chiaweng, Oxford

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Lunar soil
mechanics (started
recently)

Luc Scholtès, Brisbane

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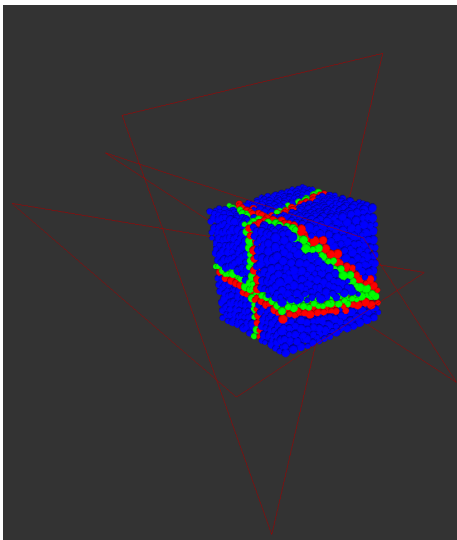
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Fractured rock
mass with smooth
contact
discontinuities;
discontinuities can
be imported from
Discrete Fracture
Network Modelers.

Luc Scholtès, Brisbane

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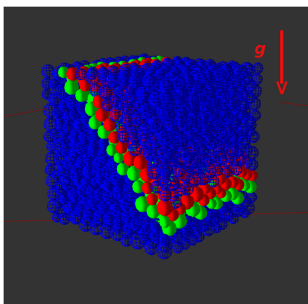
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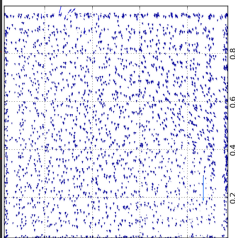
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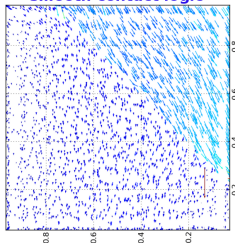


velocity field

non smooth contact logic



smooth contact logic



Fractured rock
mass with smooth
contact
discontinuities;
discontinuities can
be imported from
Discrete Fracture
Network Modelers.

Václav Šmilauer, Prague/Grenoble

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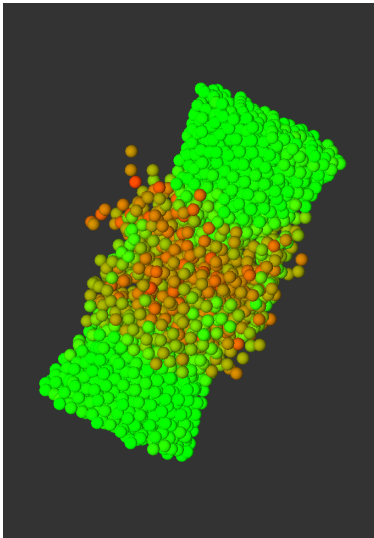
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Particle model of
concrete, based on
continuous
formulation
(plasticity,
rate-dependence,
damage).

Thanks for attention

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Got questions

