Discrete Element methods for computational mechanics

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Outline

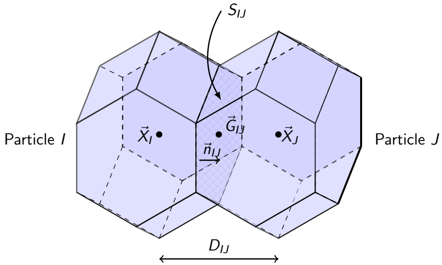
1. Discrete Element method
   - Mka3D
   - Analysis and numerical validation
   - Time-integration
   - Why use a DEM ?
2. Multiphysics coupling
   - Coupling with FEM
   - Fluid-structure interaction
3. Perspectives

Particle methods

- General principle: replace the equations of continuum mechanics by forces and torques between particles
- Solve the equations of motion for each rigid particle
- Various particle methods:
  - Smoothed Particle Hydrodynamics (SPH)
  - Particle Finite Element method (PFEM)
  - Discrete Element methods (DEM)
- Two main classes of DEMs:
  - DEMs for granular materials:
    - Particles represent physical elements (grains or crystals)
    - Spherical elements
    - Finite characteristic length
  - DEMs as discretization methods:
    - Consistency with continuous equations
    - Issue: identify the force and torque parameters from macroscopic parameters

Discrete Element method Mka3D

- Solid discretized with rigid convex polyhedral particles
- No parameter identification depending on a sphere packing
- Linear elasticity: forces and torques parametrized by Young modulus E and Poisson ratio ν
- Covers the full range of $\nu \in (-1, 0.5)$



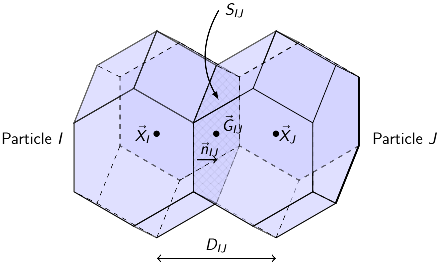
Forces between particles

- Internal force between particles : $\vec{F}_{IJ} = \vec{F}^n_{IJ} + \vec{F}^v_{IJ}$
- Shear-compression force:

$$\vec{F}^n_{IJ} = \frac{S_{IJ}}{D^0_{IJ}} \frac{E}{1+\nu} \vec{\Delta u}_{IJ}$$

- Volumetric deformation force $\vec{F}^v_{IJ}$:

$$\vec{F}^v_{IJ} = \frac{S_{IJ}}{D^0_{IJ}} \frac{E\nu}{(1+\nu)(1-2\nu)} \varepsilon_{IJ} \vec{\tilde{n}}_{IJ}$$

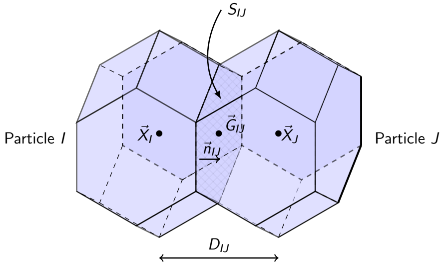


Torques between particles

- Torque of force $\vec{F}_{IJ}$: $\vec{\mathcal{M}}^t_{IJ} = \left(\mathbf{Q}_I \cdot \vec{X}^0_I \vec{G}_{IJ}\right) \wedge \vec{F}_{IJ}$
- Flexion-torsion torque :

$$\vec{\mathcal{M}}^f_{IJ} = \frac{S_{IJ}}{D^0_{IJ}}(\alpha_n(\mathbf{Q}_I \cdot \vec{n}^0_{IJ}) \wedge (\mathbf{Q}_J \cdot \vec{n}^0_{IJ}) + \alpha_s(\mathbf{Q}_I \cdot \vec{s}_{IJ}) \wedge (\mathbf{Q}_J \cdot \vec{s}_{IJ}) + \alpha_t(\mathbf{Q}_I \cdot \vec{t}_{IJ}) \wedge (\mathbf{Q}_J \cdot \vec{t}_{IJ})),$$

- Total internal torque between particles : $\vec{\mathcal{M}}_I = \sum_{J \in \tau_I} \vec{\mathcal{M}}^t_{IJ} + \vec{\mathcal{M}}^f_{IJ}$



Modified equation analysis

- We use a Cartesian lattice
- Small displacements and rotations
- We find the modified equation :

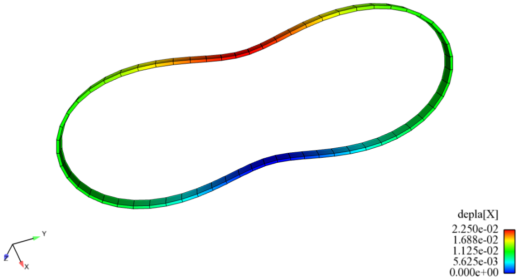
$$\rho\ddot{\vec{\xi}} = \frac{E}{1+\nu}(\Delta\vec{\xi} + \operatorname{curl}\vec{\theta}) + \frac{E\nu}{(1+\nu)(1-2\nu)}\vec{\operatorname{grad}}\operatorname{div}\vec{\xi} + \mathcal{O}(h^2)$$

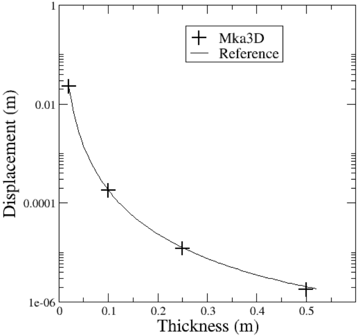
$$\frac{h^2}{6}\rho\ddot{\vec{\theta}} = \frac{E}{1+\nu}(\operatorname{curl}\vec{\xi} - 2\vec{\theta}) + \mathcal{O}(h^2)$$

- No constitutive relation between $\vec{\xi}$ and $\vec{\theta}$
- Cosserat material with characteristic length $l_c = \frac{\sqrt{2}}{2}h$
- Converges to Cauchy material as $l_c \to 0$ [Forest, Pradel, Sab, 2001]

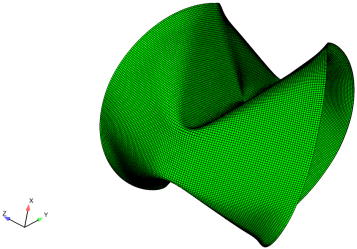
Lamb's problem

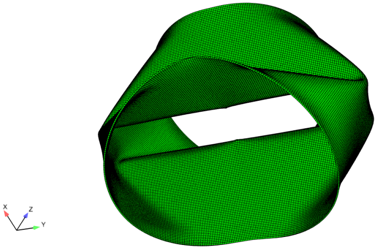
Rods and shells





Rods and shells





Time-integration scheme

- Forces and torques derived from energies: Hamiltonian formulation
- Explicit time-integration scheme: Symplectic Verlet scheme for translation and RATTLE scheme for rotation

$$\vec{V}_I^{n+\frac{1}{2}} = \vec{V}_I^n + \frac{\Delta t}{2m_I}\vec{F}_{I,\text{int}}^n, \qquad \vec{F}_{I,\text{int}} = \sum_{J\in\tau_I}\vec{F}_{IJ}$$

$$\vec{X}_I^{n+1} = \vec{X}_I^n + \Delta t\vec{V}_I^{n+\frac{1}{2}},$$

$$\mathbf{P}_I^{n+\frac{1}{2}} = \mathbf{P}_I^n + \frac{\Delta t}{4}\mathbf{j}(\vec{\mathcal{M}}_{I,\text{int}}^n)\mathbf{Q}_I^n + \frac{\Delta t}{2}\boldsymbol{\Upsilon}_I^n\mathbf{Q}_I^n, \qquad \boldsymbol{\Upsilon}_I^n \text{ s.t } (\mathbf{Q}_I^{n+1})^t\mathbf{Q}_I^{n+1} = \mathbf{I},$$

$$\mathbf{Q}_I^{n+1} = \mathbf{Q}_I^n + \Delta t\mathbf{P}_I^{n+\frac{1}{2}}\mathbf{D}_I^{-1},$$

$$\vec{V}_I^{n+1} = \vec{V}_I^{n+\frac{1}{2}} + \frac{\Delta t}{2m_I}\vec{F}_{I,\text{int}}^{n+1},$$

$$\mathbf{P}_I^{n+1} = \mathbf{P}_I^{n+\frac{1}{2}} + \frac{\Delta t}{4}\mathbf{j}(\vec{\mathcal{M}}_{I,\text{int}}^{n+1})\mathbf{Q}_I^{n+1} + \frac{\Delta t}{2}\tilde{\boldsymbol{\Upsilon}}_I^{n+1}\mathbf{Q}_I^{n+1},$$

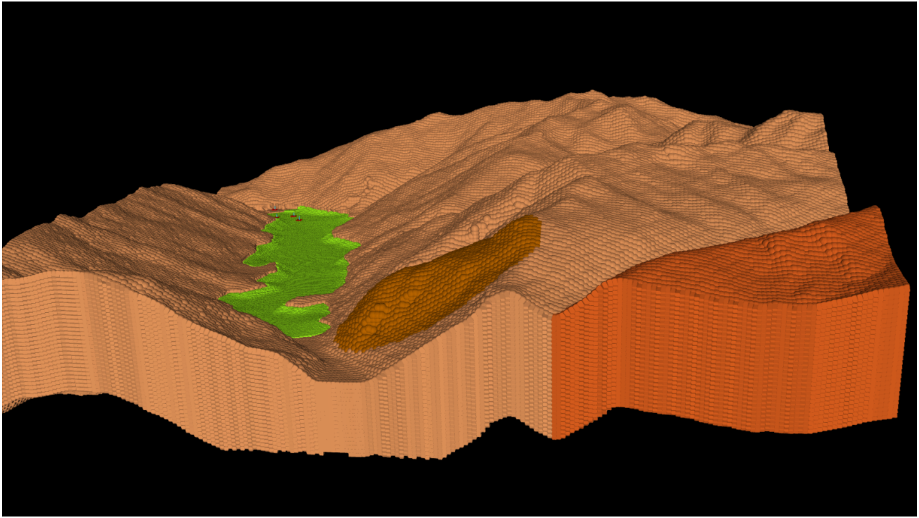
$$\tilde{\boldsymbol{\Upsilon}}_I^{n+1} \text{ s.t } (\mathbf{Q}^{n+1})^t\mathbf{P}^{n+1}\mathbf{D}^{-1} + \mathbf{D}^{-1}(\mathbf{P}^{n+1})^t\mathbf{Q}^{n+1} = \mathbf{0}$$

- CFL condition on Δt

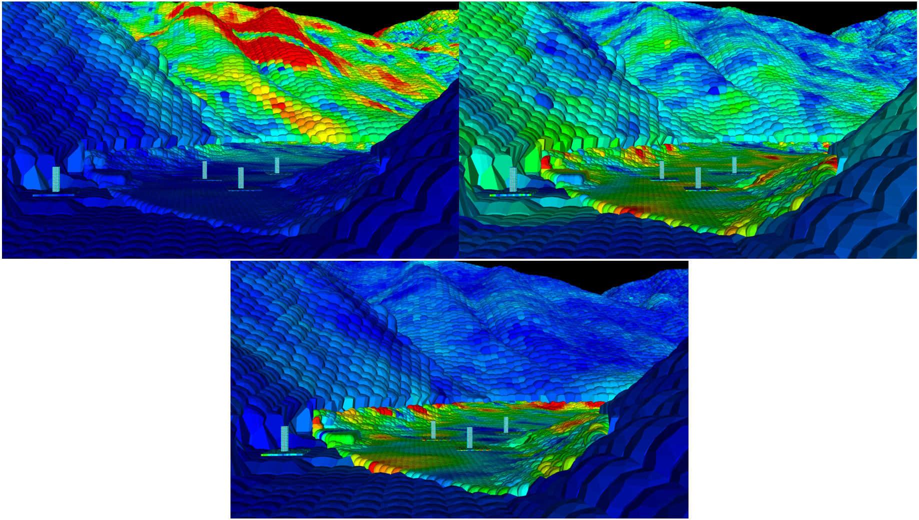
Why use a Discrete Element method ?

- Well-adapted to fast dynamics (impact, fragmentation)
- Simple handling of fracture
- Versatility: seismic wave propagation, rods and shells in a single framework
- Parallelization
- Difficulties:
  - Time-consuming
  - Integration of continuum equations in the formulation: PhD F. Marazzato for ductile fracturation (advisors: A. Ern, K. Sab, C. Mariotti, LM)
  - Analysis on general polyhedral meshes: comparison with CDO schemes (J. Bonelle, A. Ern)

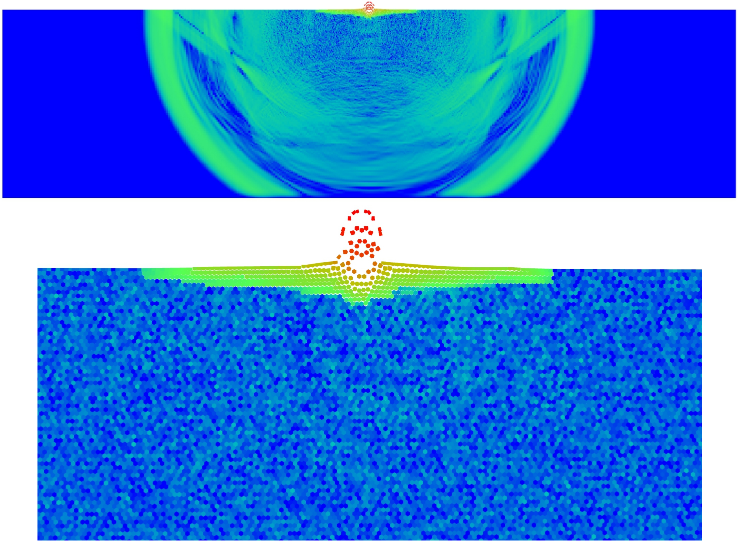
Seismic propagation in a sedimentary valley



Seismic propagation in a sedimentary valley



Coupling with a Spectral Element Method (SEM)



Coupling with a Spectral Element Method (SEM)

- Explicit coupling of SEM with DEM
- Displacement of SEM interpolated on interface particles (w/o rotation)
- Load transferred from DEM to SEM boundary conditions (least-square)
- Energy balance
- Possible improvements:
  - Take into account rotation: better transmission of Rayleigh surface waves
  - Allow for different time-steps for SEM and DEM

Fluid-structure interaction

- Risk prevention (effects of an explosion on a structure)
- Interaction between a shock wave and a moving structure
- Effect of overpressure and possible effect of fragments
- Fluid: Eulerian Finite Volume method for Navier-Stokes (OSMP flux [Daru, Tenaud 2004])
- Globally explicit coupling
- Conservation of mass, momentum and energy of the coupled system
- Large displacements and possible fragmentation

  $\Rightarrow$ *Avoid ALE (remeshing involved) and choose Immersed Boundaries*

Deformed boundary reconstruction

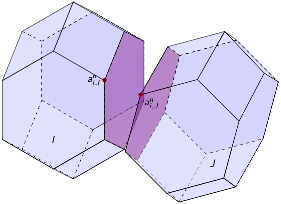


Figure 1: Solid deformation

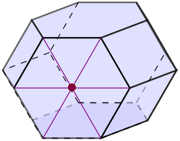


Figure 2: Triangulated face

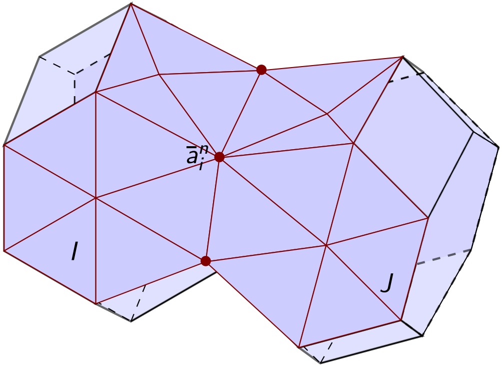


Figure 3: Deformed boundary reconstruction

$$\bar{a}_i^n = \frac{1}{\#\mathcal{P}_{a_i}} \sum_{I \in \mathcal{P}_{a_i}} \left(\vec{X}_I^n + \mathbf{Q}_I^n \cdot (a_{i,I}^n - \vec{X}_I^0)\right)$$

Cut-cells description

- Investigated for rigid bodies by Noh (1964), Colella *et al.* (1995), ...
- Volume fraction $0 \leqslant \Lambda \leqslant 1$ occupied by the solid in the cell
- Side area fraction $0 \leqslant \lambda \leqslant 1$ of each face
- Boundary area A and exterior normal vector $\vec{n}$

$\Rightarrow$ Intersection between 3d objects: geometric library CGAL (INRIA et al.)

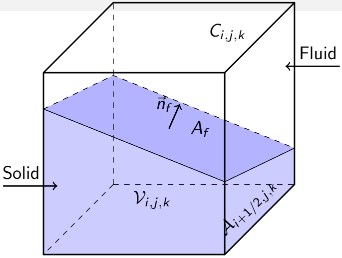


Figure 4: Cut cell

$$\left(1-\Lambda_{i,j,k}^{n+1}\right) U_{i,j,k}^{n+1} = \left(1-\Lambda_{i,j,k}^{n+1}\right) U_{i,j,k}^{n} + \Delta t \left(\frac{\left(1-\lambda_{i-1/2,j,k}^{n+1}\right)}{\Delta x_{i,j,k}} F_{i-1/2,j,k}^{n} - \frac{\left(1-\lambda_{i+1/2,j,k}^{n+1}\right)}{\Delta x_{i,j,k}} F_{i+1/2,j,k}^{n} + \cdots \right)$$

$$+ \frac{\Delta t}{V_{i,j,k}} \sum_{\{f \mid f^{n+1} \subset C_{i,j,k}\}} \phi_f^n + \sum_{\{f \mid f^{n+1} \subset C_{i,j,k}\}} \Delta U_f^{n,n+1}$$

ϕ_f: action of the solid on the fluid $\quad \Delta U_f^{n,n+1}$ - amount of U^n swept by f between n and $n+1$

[M. A. Puscas, LM 2015]

Fragmenting solid

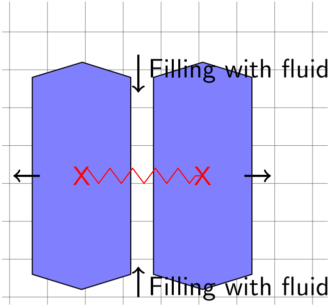


Figure 5: Breaking the link between two particles

⇒ Vacuum between solid particles if the velocity of the crack propagation is larger than the speed of sound in the fluid

⇒ Fluid cells with fluid pressure and density close to zero

⇒ Solve the Riemann problem in the presence of vacuum

- Lax-Friedrichs flux near the vacuum area
- Progressive filling

[M. A. Puscas, LM, A. Ern, C. Tenaud, C. Mariotti 2015]

Explicit time integration scheme

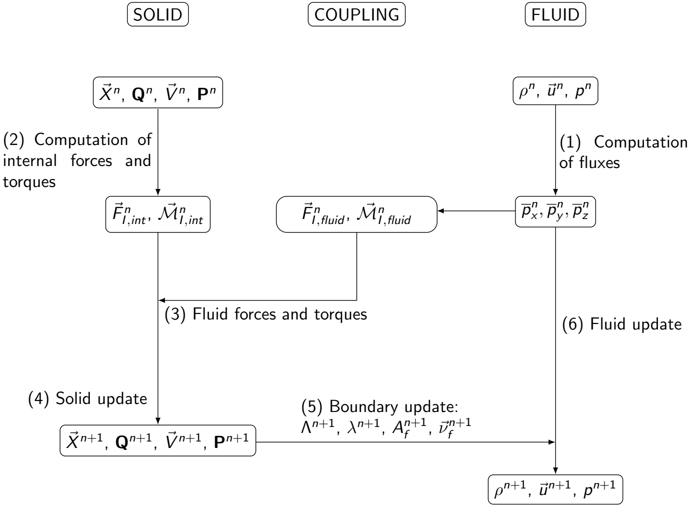
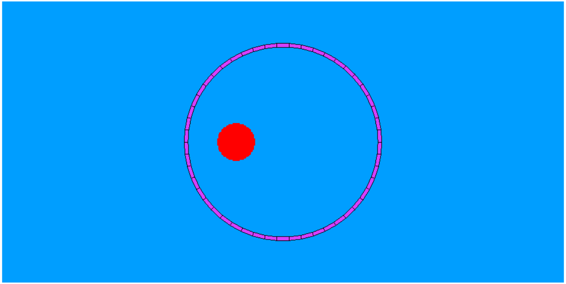


Figure 6: Structure of the explicit coupling scheme

Effects of an explosion on an steel cylinder in 2d

Fluid: $\rho_F = 99.9\text{kg.m}^{-3}$, $p = 50662500\text{Pa}$ (~ 100kg TNT)
Solid: $\rho_S = 7860\text{kg.m}^{-3}$, $E = 210\text{GPa}$, $\nu = 0$.
Fluid grid: 600×300 and solid: 50 particles along circumference and 1 particle in thickness.



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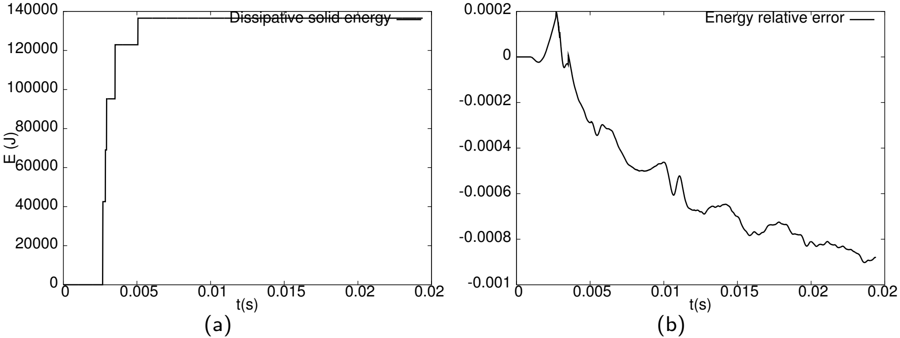

Figure 7: (a) Dissipative energy and (b) Relative conservation error on system energy.

Perspectives

- Ductile fragmentation vs fragile fragmentation (F. Marazzato)
- Improvement of the time-integration scheme with variable time-steps
- Integration of contact in the fluid-structure coupling scheme

References

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