One application of the MGIS project to a variational problem modelling a damaged elasto-plastic material

Fifth MFront User Meeting

Goustan Bacquaert

École des Ponts ParisTech/Sorbonne Université

EDF Lab Paris Saclay

November, 25th 2020

Outline

1. Framework and objectives
2. MFront integration of the local model
3. MGIS usefulness for developing a regularized model
4. Perspectives

1. Framework and objectives
   - Experimental observations on granular materials
   - Work basing support
2. MFront integration of the local model
   - From the local formulation to the MFront vocabulary
   - A need to regularize the local model
3. MGIS usefulness for developing a regularized model
   - A regularisation by the damage gradient
   - The Algorithmic strategy
   - Numerical applications
4. Perspectives

At the macroscopic scale

A key-vocabulary to describe the experimental observations:

- Hardening and softening behaviours.
- Contractancy and dilatancy behaviours.
- Critical state.

+ Typical evolutions with cyclic loads, hydro-mechanical coupling, etc.

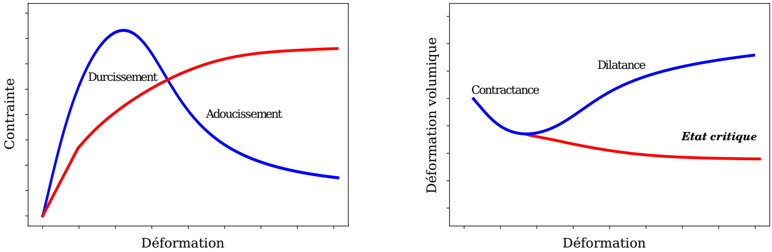


FIG.: Two possible stress and volumetric strain responses for a dense or loose sand

At the microscopic scale

Use of digital image correlations to visualize the mechanical transformations at the grain level ($\sim 10^{-4} - 10^{-2}$ mm):

- Heterogeneous strain field.
- Shear bands growth.
- High levels of porosity.

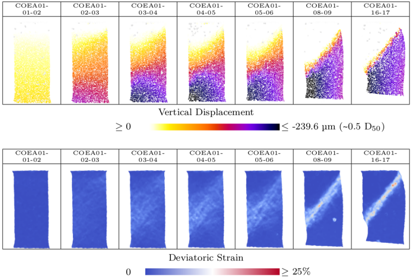


FIG.: Visualization of displacement and strain localisations from a simple compression test[1]

1. Desrues, J. and Andò, E., Strain localisation in granular media, Comptes Rendus Physique, 2015

Framework of the model development

Context: 6 months of Master internship, at EDF Lab[2], with SU and ENPC[3] supports.
Initial feed: a generalised standard material (GSM) model coupling plasticity with damage[4].

Summarized ideas

Sound elasticity with damaged kinematic hardening:

$$\psi\left(\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}^{\boldsymbol{p}},\alpha\right) = \psi_e\left(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{\boldsymbol{p}}\right) + \psi_h\left(\boldsymbol{\varepsilon}^{\boldsymbol{p}},\alpha\right)$$

$$\psi_e\left(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{\boldsymbol{p}}\right) = \frac{1}{2}\left(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{\boldsymbol{p}}\right) : \mathbb{C} : \left(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{\boldsymbol{p}}\right) \quad ; \quad \psi_h\left(\boldsymbol{\varepsilon}^{\boldsymbol{p}},\alpha\right) = \frac{1}{2}\boldsymbol{\varepsilon}^{\boldsymbol{p}} : \mathbb{H}\left(\alpha\right) : \boldsymbol{\varepsilon}^{\boldsymbol{p}}$$

Linear superposition of Drucker-Prager and Griffith dissipations:

$$\varphi\left(\dot{\boldsymbol{\varepsilon}}^{\boldsymbol{p}},\dot{\alpha}\right) = \frac{\sigma_0}{k}\dot{\varepsilon}_v^p + \mathrm{D}_1\dot{\alpha}$$

2. Alves Fernandes, V. Raude, S. and Voldoire, F., Département ERMES

3. Kondo, D. and Maurini, C., Laboratoire D'Alembert, Bleyer, J., Laboratoire Navier

4. Marigo, J.-J. and Kazymyrenko, K., A micromechanical inspired model for the coupled to damage elasto-plastic behavior of geomaterials under compression, Mechanics & Industry, 2019

1. Framework and objectives
    - Experimental observations on granular materials
    - Work basing support

2. MFront integration of the local model
    - From the local formulation to the MFront vocabulary
    - A need to regularize the local model

3. MGIS usefulness for developing a regularized model
    - A regularisation by the damage gradient
    - The Algorithmic strategy
    - Numerical applications

4. Perspectives

Pseudo-code

Behaviour	Thermodynamic force	Criterium
Plasticity	$\boldsymbol{X} = \boldsymbol{\sigma} - \mathbb{H}\left(\alpha\right) : \boldsymbol{\varepsilon^p}$	$f_p(\boldsymbol{X}) = X_{eq} + kX_m - \sigma_0 \leq 0$
Damage	$Y = -\frac{1}{2}\boldsymbol{\varepsilon^p} : \mathbb{H}'\left(\alpha\right) : \boldsymbol{\varepsilon^p}$	$f_d\left(Y\right) = Y - \mathrm{D}_1 \leq 0$

MFront outline

1. Elastic prediction $\left(\Delta\boldsymbol{\varepsilon^p} = 0, \Delta\alpha = 0\right)$:

$$f_p\left(\boldsymbol{\varepsilon} + \Delta\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon^p}, \alpha\right) \leq 0$$

2. If $f_p > 0$ plastic correction $(\Delta\varepsilon^p \neq 0, \Delta\alpha = 0)$:

$$f_p\left(\boldsymbol{\varepsilon} + \Delta\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon^p} + \Delta\boldsymbol{\varepsilon^p}, \alpha\right) = 0 \quad ; \quad f_d\left(\boldsymbol{\varepsilon^p} + \Delta\boldsymbol{\varepsilon^p}, \alpha\right) \leq 0$$

3. If $f_d > 0$ damage correction $\left(\Delta\boldsymbol{\varepsilon^p} \neq 0, \Delta\alpha > 0\right)$:

$$f_p\left(\boldsymbol{\varepsilon} + \Delta\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon^p} + \Delta\boldsymbol{\varepsilon^p}, \alpha + \Delta\alpha\right) = 0 \quad ; \quad f_d\left(\boldsymbol{\varepsilon^p} + \Delta\boldsymbol{\varepsilon^p}, \alpha + \Delta\alpha\right) = 0$$

Numerical responses vs available data

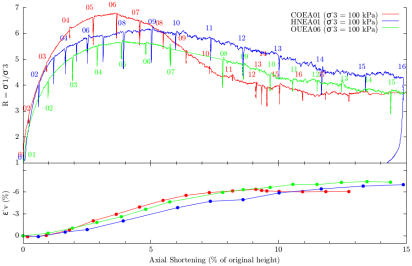


FIG.: Simple compressive test response on dense sands[1]

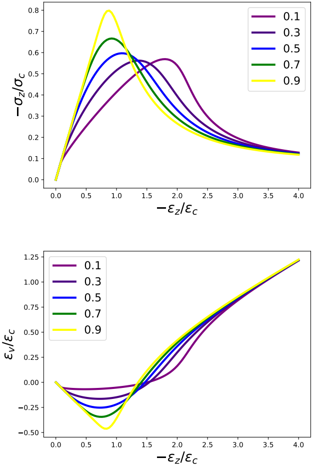


FIG.: Some parametric studies (mtest)

Numerical pathologies from the softening behaviour

Damage responsible for a softening behaviour, incompatible with a well-posed model:

- Field localisation on one element in finite element simulations.
- Mesh dependency (band size and orientation, level of dissipation).
- Mistrust of the numerical results.

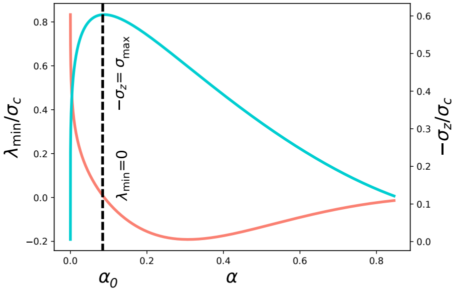
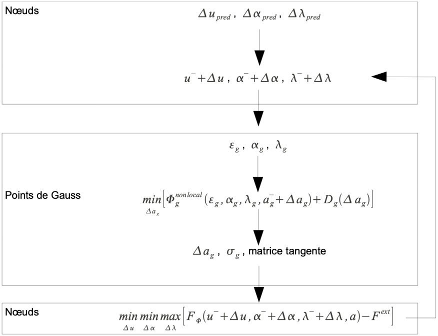


FIG.: Hill unicity criterium at the integration point ($\lambda_{\min}$ minimal eigenvalue of $\mathbb{C}_{\text{tg}}$)

Regularisation at EDF

Available technique to regularize purely damage (without plasticity) model in Code_Aster by constructing a non-local one by adding the internal variable gradient. Concisely [5]:

- The internal variable a is defined at the integration points.
- It must be duplicate by α defined at the nodes to have access to its gradient.
- Lagrange multipliers λ to constrain $\alpha = a$ are thus introduced.



FEniCS: internal variable directly defined at nodes, no need of duplication. Strategy privileged in the internship to study one proposed regularized model.

5. Kazymyrenko, K., Modélisation non locale à gradients de variables internes GRAD_VARI, 2011

1. Framework and objectives
   - Experimental observations on granular materials
   - Work basing support
2. MFront integration of the local model
   - From the local formulation to the MFront vocabulary
   - A need to regularize the local model
3. MGIS usefulness for developing a regularized model
   - A regularisation by the damage gradient
   - The Algorithmic strategy
   - Numerical applications
4. Perspectives

New variational formulation

Global potential defined on the structure Ω, with the introduction of the damage gradient correlated to an intrinsic length l.

$$\Psi\left(\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}^{p},\alpha\right)=\int_{\Omega}\psi\left(\boldsymbol{\varepsilon}\left(\underline{x}\right),\boldsymbol{\varepsilon}^{p}\left(\underline{x}\right),\alpha\left(\underline{x}\right)\right)\mathrm{d}\Omega$$

$$\Phi\left(\dot{\boldsymbol{\varepsilon}}^{p},\dot{\alpha}\right)=\int_{\Omega}\varphi\left(\dot{\boldsymbol{\varepsilon}}^{p}\left(\underline{x}\right),\dot{\alpha}\left(\underline{x}\right)\right)\mathrm{d}\Omega+\mathrm{D}_1 l^2\int_{\Omega}\underline{\nabla}\alpha\left(\underline{x}\right).\underline{\nabla}\dot{\alpha}\left(\underline{x}\right)\mathrm{d}\Omega$$

$$\mathcal{E}=\Psi\left(\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}^{p},\alpha\right)+\int_{0}^{t}\Phi\left(\dot{\boldsymbol{\varepsilon}}^{p},\dot{\alpha}\right)\mathrm{d}t-\mathcal{W}_{\mathrm{ext,d}}$$

Regularisation inspired by phase-field models applied to brittle fracture problem. Similar applications to another damage/plasticity coupling can be found [6]. Minimising $\mathcal{E}$ according to the three involved fields (in some appropriate spaces) enable to compute a mechanical consistent solution (respecting equilibrium equation, plastic and damage criteria).

6. Alessi, R. Marigo J.-J. and Vidoli, S., Gradient damage models coupled with plasticity: Variational formulation and main properties, Mechanics of Materials, 2015

An efficient interaction between MFront and FEniCS

The mechanical problem is divided into two sub-problems, handled by MFront and FEniCS environments, connected thanks to the MGIS project.

1. Resolution of the local equations with damage α fixed under MFront, on the fields of displacement $\underline{u}$ and plastic strain $\boldsymbol{\varepsilon^p}$. The integrator handles only a **linear kinematic hardening behaviour**.
2. Damage minimization under FEniCS. Optimization under constraints ($\dot{\alpha} > 0$) of a **convex functional** with a TA0 solver:

$$\mathcal{E}_{\mathrm{obj}}\left(\alpha\right) = \int_{\Omega}\left(\frac{1}{2}\boldsymbol{\varepsilon^p}\left(\underline{x}\right) : \mathbb{H}\left(\alpha\left(\underline{x}\right)\right) : \boldsymbol{\varepsilon^p}\left(\underline{x}\right) + \mathrm{D}_1\left(\alpha\left(\underline{x}\right) + \frac{l^2}{2}\left\|\underline{\nabla}\alpha\left(\underline{x}\right)\right\|^2\right)\right)\mathrm{d}\Omega$$

Remarks:

- Well-posed MFront/FEniCS sub-problems to compute a mesh-independent solution verifying the mechanical equations.
- Which sub-problem is the most time-consuming? From numerical experiments, the α-minimization one.

Pseudo-code

Resolution at the load step i

⋆ Initialisation with the previous solution at $i-1$:

$$\underline{u}^{(i,0)} = \underline{u}^{(i-1)} \quad ; \quad \boldsymbol{\varepsilon}^{\boldsymbol{p},(i,0)} = \boldsymbol{\varepsilon}^{\boldsymbol{p},(i-1)} \quad ; \quad \alpha^{(i,0)} = \alpha^{(i-1)}$$

1. MFront sub-problem on $\underline{u}^{(i,k+1)}$ and $\boldsymbol{\varepsilon}^{\boldsymbol{p},(i,k+1)}$:

$$f_p\left(\boldsymbol{\varepsilon}\left(\underline{u}^{(i,k+1)}\right), \boldsymbol{\varepsilon}^{\boldsymbol{p},(i,k+1)}, \alpha^{(i,k)}\right) \leq 0$$

2. FEniCS sub-problem on $\alpha^{(i,k+1)}$:

$$\alpha^{(i,k+1)} = \underset{\alpha^{(i-1)} \leq \alpha \leq 1}{\arg\min} \; \mathcal{E}_{\mathrm{obj}}^{(i,k+1)}(\alpha)$$

⋆ Iteration on k until convergence (on $\|\alpha^{(i,k+1)} - \alpha^{(i,k)}\|_\infty$ for instance):

$$\underline{u}^{(i)} = \underline{u}^{(i,k+1)} \quad ; \quad \boldsymbol{\varepsilon}^{\boldsymbol{p},(i)} = \boldsymbol{\varepsilon}^{\boldsymbol{p},(i,k+1)} \quad ; \quad \alpha^{(i)} = \alpha^{(i,k+1)}$$

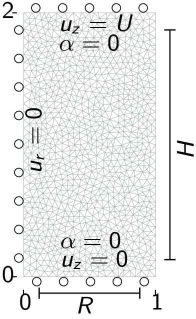
Translation in python

Shortly in a notebook (Remark: $d = \alpha$):

```python
# Material definition (properties, behaviour, hypothesis)
material = mf.MFrontNonlinearMaterial("../materials/src/libBehaviour.dylib",
                                      "MK_law",
                                      hypothesis="axisymmetric",
                                      material_properties=mat_prop)

# Definition of the 1 sub-problem (at the damage fixed)
problem_1 = mf.MFrontNonlinearProblem(u, material, quadrature_degree=2, bcs=bcu)
problem_1.register_external_state_variable("Damage", d)

# Definition of the 2 sub-problem (relative to the damage)
problem_2 = PETScTAOSolver()


# At each load step, the alternated minimisation is called
def alternate_minimization(u, d, tol=1e-5, Nitermax=500):

    for niter in range(Nitermax):

        problem_1.solve(u.vector())
        problem_2.solve(DamageProblem(), d.vector(), dlb.vector(), dub.vector())

        Res = max(d.vector().get_local()-dold.vector().get_local())
        dold.assign(d)

        if nRes < tol:
                break

    dlb.assign(d)
```

Macroscopic responses on axisymmetric tests

material = mf.MFrontNonlinearMaterial(...,hypothesis='axisymmetric')



- Displacement: $\mathcal{P}_2$.
- Damage: $\mathcal{P}_1$.

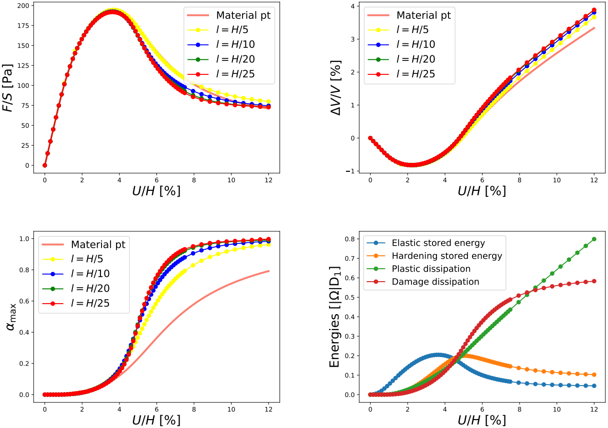


FIG.: Macroscopic responses according to l

Plastic and damage fields

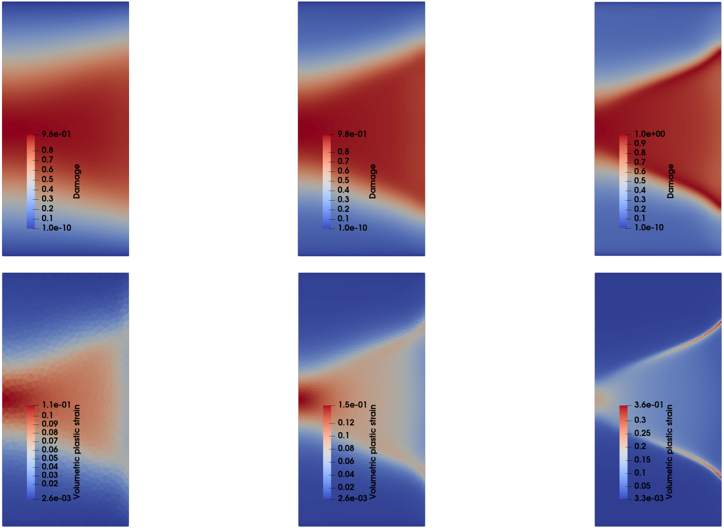
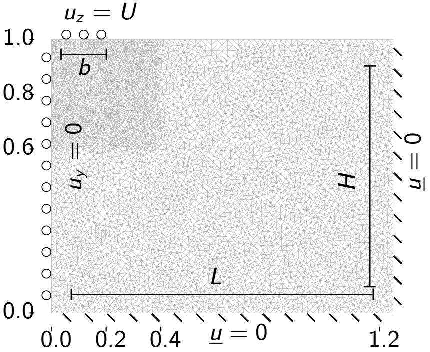
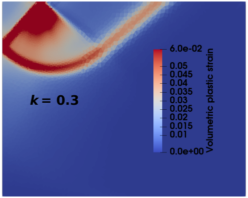


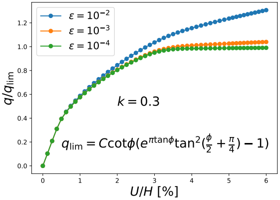
FIG.: Final damage and plastic fields ($U/H = 12\%$) for $l = H/5, H/10$ et $H/25$

Toward more interesting simulations

material = mf.MFrontNonlinearMaterial(...,hypothesis='plane_strain')







Limit analysis: $q_{\lim} = C\cot\phi\left(e^{\pi\tan\phi}\tan^2\left(\frac{\phi}{2}+\frac{\pi}{4}\right)-1\right)$
Residual hardening: $\psi_h(\boldsymbol{\varepsilon^p}) = \frac{1}{2}\epsilon E_0\|\boldsymbol{\varepsilon^p}\|^2$

Numerical observations

$\mathbb{H}_\epsilon \leftrightarrow \mathbb{H}(\alpha)$. What difference can be expected?

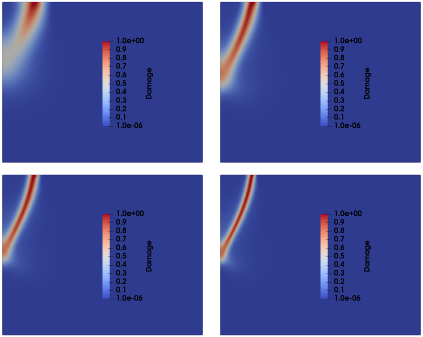
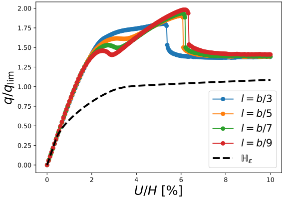
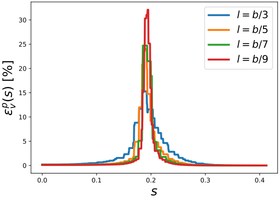


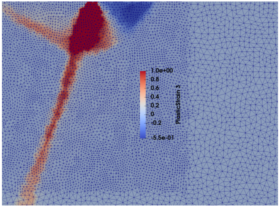
FIG.: Damage field at $U/H = 4\%$ according to l





Numerical observations

Results raising interesting comments:



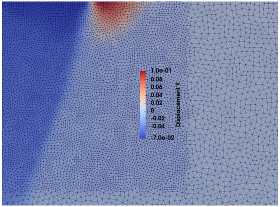


FIG.: ε^p_{yz} and u_z fields at the maximal load ($U/H = 10\%$)

- The length l localizes the plastic strains before a breakdown appears, then a Prantdl mechanism is approached.
- The Young modulus E_0 influences the asymptotic charge. Different from limit analysis.

1. Framework and objectives
   - Experimental observations on granular materials
   - Work basing support
2. MFront integration of the local model
   - From the local formulation to the MFront vocabulary
   - A need to regularize the local model
3. MGIS usefulness for developing a regularized model
   - A regularisation by the damage gradient
   - The Algorithmic strategy
   - Numerical applications
4. Perspectives

Coming work

Enrichment of the local model to take into account cyclic and undrained behaviours (with fluid interaction). Not an easy task since:

1. Proposing a cyclic model respecting GSM principles relevant to soils is not an easy task.
2. Adding fluid interaction entails issues of stability which should be carefully considered.

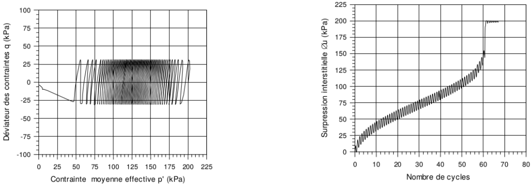


FIG.: Fluid pressure and stress responses from an undrained simple compression of a loose sand[7]

Transposition of the finally adopted model to Code_Aster. Ultimate goal aimed at the end of the Cifre thesis collaborating EDF, ENPC and SU (2020-2023).

7. Canou, J., Instabilités de liquéfaction et phénomène de mobilité cyclique dans les sables, Rev. Fr. Geotech., 2002