Simulation of localized compaction in high-porosity calcarenite subjected to boundary constraints

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This paper studies the mechanics of localized compaction in porous rocks subjected to axisymmetric deformation. The material selected for the study is Gravina calcarenite, a soft rock prone to pore collapse and compaction banding. The stress–strain response has been simulated through a plasticity model capturing inelastic processes in the brittle–ductile transition, while the bifurcation theory has been used to calibrate the model constants and identify stress paths able to generate heterogeneous compaction. The onset of strain localization upon application of the selected paths has been assessed numerically, simulating the global response of calcarenite specimens via the Finite Element Method. Simulated triaxial compression tests have been compared with published experiments, showing good agreement in terms of both macroscopic response and localization patterns. In addition, oedometric compression has been simulated to inspect the role of material heterogeneity, kinematic constraints and boundary effects. The results show that the interplay between these factors has important implications for the resulting localization process. In particular, heterogeneity and boundary conditions have been found to control the formation of unexpected strain patterns, such as compactive shear zones that do not reappear with further strains and the averaging of the quantities measured at the boundary tends to disappear with further strains and the averaging of the quantities measured at the boundary tends to generate global signatures not easily distinguishable from those associated with pure (horizontal) compaction banding.

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1. Introduction

High-porosity rocks display a wide range of localization mechanisms controlled by microstructural attributes and stress conditions [1]. In particular, when such rocks are loaded at high confinements they tend to exhibit compaction bands orthogonal to the maximum compressive stress [2–5]. These modes of localization have attracted the interest of different communities, such as structural geology, geophysics, geotechnical and petroleum engineering. This interest is motivated by the ability of these structures to reduce the permeability of reservoir rocks and threaten the stability of deep boreholes [6,7]. After being identified in the field by Mollema and Antonellini [8], the mechanisms leading to the formation of compaction bands have been studied via laboratory tests [2–4,9–14], theoretical investigations [15–20] and numerical analyses [21–25]. These studies, together with microstructural inspections, identified grain crushing and pore collapse as the key micromechanical processes that control the formation of compaction bands. While these processes induce a local loss of strength, they also increase the frequency of intergranular contacts, thus promoting the rearrangement of the crushed fragments, the reduction of the local porosity and the re-hardening of the post-localization regime. As a result, unlike single shear bands observed at low confinements, the brittle–ductile regime promotes multiple compaction zones that propagate across the sample until a complete re-hardening of the specimen [26].

The systematic observation that compaction bands tend to form in such a peculiar regime of deformation has inspired testing procedures based on pre-selected triaxial compression paths, i.e., stress paths designed to pass through the transitional regime of the tested rock [2,3,13]. While these methods have disclosed important characteristics of compaction banding, the conditions imposed in the laboratory may significantly differ from those occurring in the field [27,28]. For example, recent experiments have pointed out the importance of anisotropic stress paths for the onset of strain inhomogeneities [29,30], while theoretical studies have suggested that non-axisymmetric loading [31] and kinematic constraints [32] may hinder the formation of compaction bands. Insights on this matter have been recently provided by Soliva et al. [33], who discussed the effect of...
factors such as burial history and local tectonics on stress paths and consequent strain localization mechanisms.

It is therefore arguable that the theoretical/numerical inspection of different kinematic conditions and stress paths is a valuable tool to improve the understanding of compaction bands and identify the key processes that control their formation in the field. For these reasons, here we study the relation between the axisymmetric stress paths that derive from imposed kinematic constraints and the onset of compaction banding. In particular, numerical modeling will be used to explore the influence of kinematic conditions, boundary restraints and material heterogeneity. The reference material selected for the study is Gravina calcarenite, a porous rock from Southern Italy prone to pore collapse, degradation of its cement matrix and strain inhomogeneities [14,34–36].

The study consists of two distinct parts. In the first one, the constitutive response of the selected soft-rock is simulated through an elasto-plastic model developed by Nova and co-workers [35,37,38], which has been chosen for its ability to capture inelastic mechanisms in the brittle–ductile transition. The model predictions are then inspected via a bifurcation criterion for strain localization [39], identifying a set of stress paths able to generate localized compaction. In the second part, numerical simulations are used to model the response of calcarenite specimens as boundary value problems. The objective of the numerical study is to inspect onset and propagation of localized compaction and elucidate the role of imposed kinematic constraints. For this purpose, a Finite Element model enriched with a rate-dependent regularization scheme [40,41] has been used to reproduce triaxial compression and oedometric compaction in presence of different boundary conditions. The computed response is finally compared with experimental data, discussing the interplay between the imposed conditions and the predicted patterns of heterogeneous compaction.

2. Constitutive analysis of localized compaction

2.1. Constitutive model for porous rocks

An essential component for compaction band analyses is a constitutive law able to replicate the rheological response of specimens loaded in the brittle–ductile transition zone, as well as to capture the associated strain localization processes. A popular strategy involves the use of cap plasticity [42], which allows the simulation of inelastic compaction during compression. While parabolic cap models [43] and elliptic caps [42] are typical choices, numerous enhancements have been proposed in recent years to better fit the data [44,45]. Another option for constitutive analyses is critical state plasticity [46,47], which links the stress–strain response to the evolving plastic volumetric strains. Despite these features, cap plasticity and critical state theories have been typically used to assess the potential for localized compaction at yielding [45,48,49], and only few studies have considered the interplay between stress–strain response and patterns of localized compaction [22,24,50]. In addition, most of the existing works do not include a description of the irreversible processes that control the mechanics of compaction, such as bond/grain breakage and pore collapse. A notable exception is the work by Das et al. [16,21], in which the explicit incorporation of grain crushing allowed the authors to point out the importance of the rheological response on the simulation of both onset and propagation of compaction bands.

Here we use a similar logic, in that we use a constitutive law able to reproduce realistically the rheology of porous rocks observed in experiments. The selected model derives from a series of contributions by Nova and co-workers [35,38,51,52], and is here chosen for its ability to capture the transition from brittle to ductile behavior in a wide range of porous geomaterials [14,32,35].

At variance with typical models, this law includes multiple internal variables mimicking a number of inelastic processes involved in compaction banding (i.e., rupture of microstructural compounds and subsequent pore collapse, as well as compaction hardening). A major advantage of this strategy is the possibility to naturally reproduce the porosity loss generated by the degradation of the cement, which is captured by the plastic compensatory mechanism created by the competition between an internal variable that increases with compaction (thus mimicking a denser skeleton packing) and a second term that decreases (thus reflecting a strain-induced degradation of the microstructure, [35]). Experimental and theoretical studies have demonstrated the ability of this model to capture the macroscopic signatures of compaction banding upon oedometric compaction [53], while a recent study by Buscarnera and Laverack [32] has discussed the possibility to use it for capturing localized compaction in both porous sandstones and carbonate rocks subjected to triaxial compression.

Hereafter we provide a brief description of the constitutive formulation, focusing on the functions that allow the incorporation of non-normality. In particular, the yield function and the plastic potential are assumed to be given by the expressions proposed by Lagioia et al. [37]:

\[
\begin{align*}
 f &= A_h^{1/n_C} B_h^{-K_m/G_m} p^* - p^*_{th} = 0 \\
 A_h &= 1 + \frac{q}{K_{th} M_h} p^* \\
 B_h &= 1 + \frac{q}{K_{th} M_h} p^* \\
 K_{th/2h} &= \mu_h (1 - \mu_h) \alpha_h (1 - \mu_h) \\
 C_h &= (1 - \mu_h) (K_h - K_{th}) \\
 M_h &= \frac{2 M_{th} C_{th} \psi_{th}}{1 + C_{th} - (1 - C_{th}) \sin (3 \theta)}
\end{align*}
\]

where \(p^* = p^* + p_m = \sigma_3 / 3 + p_m\) is a modified mean effective stress; \(q = \sqrt{(3/2) \kappa_m \kappa_3}\) is the deviatoric stress (\(\kappa_3 = \sigma_3 - p_m\)) and the subscript \(h\) indicates either the yield function (\(h = f\)) or the plastic potential (\(h = g\). The size of the elastic domain (\(p_{th}^*\)) is measured along the hydrostatic axis (Fig. 1c) and is defined by a linear combination of independent internal variables, here referred to as \(p_s\) and \(p_m\) (i.e., by \(p_s = p_s + p_m + p_m\), where the term \(p_m\) represents the hydrostatic yield threshold in the tensile stress regime).

As summarized by Eqs. (1)–(5), independent parameters are needed to reproduce non-associated plastic flow. In particular, the shape of yield surface and plastic potential is defined by two sets of four parameters (\(\alpha_h, \mu_h, M_{th}\) and \(M_{ch}\)). The constants \(\alpha_h\) and \(\mu_h\) control the shape of the surfaces in meridian sections of the stress space (Fig. 1c), while \(M_{th}\) and \(M_{ch}\) control the geometry of the surfaces in the region of compression and extension loading, respectively. In particular, the ratio \(\psi_{th} = M_{th}/M_{ch}\) defines the shape of the deviatoric section (Fig. 1b), which is expressed as a function of the Lode angle, \(\theta\), according to Eq. (6) [54]. These two sets of parameter must be calibrated based on experiments, thus defining the shape of the yield surface from observed yielding points, and that of the plastic potential from the irreversible strain increments measured in the post-yielding regime [32]. The typical shape of the initial yield envelope in the principal stress space and deviatoric plane is presented in Fig. 1.

The most notable features of the model are embedded in the hardening laws [51,52]. Indeed, unlike conventional critical state
models, size and location of the yielding locus are controlled by the evolution of the internal variables, \( p_c \) and \( p_m \) (Fig. 1c), which simulate the hardening/softening response driven by compactive/dilative plastic strains and the strain-softening driven by the loss of structure due to the breakup of the microstructural compounds (e.g., cement bridges, particles, etc.), respectively. These two internal variables are coupled, in that they evolve simultaneously as a function of the plastic strains:

\[
p_c = \frac{B_p \sigma^p_c}{B_p}
\]

\[
p_m = -\rho_m p_m (\sigma^p_{ij} + \xi_m \sigma^p)
\]

where \( B_p \) is a material constant that controls the rate of compaction hardening, as well as the plastic compressibility under hydrostatic compression, while \( \rho_m \) and \( \xi_m \) govern the rate of material degradation and introduce strain-softening terms into the formulation.

The plastic strains are eventually obtained by incorporating the above mentioned constitutive functions in the plastic flow rule, as follows

\[
\dot{\varepsilon}^p_{ij} = \Lambda \frac{\partial g}{\partial \sigma^p_{ij}}
\]

where \( \Lambda \) is a non-negative plastic multiplier determined from the consistency condition.

The model is completed by defining the elastic response inside the yield envelope. For the sake of simplicity, a linear elastic relationship is used hereafter

\[
\sigma^e_{ij} = D_{ijkl} \varepsilon^e_{kl}
\]

where \( \sigma^e_{ij} \) is the Cauchy stress tensor; \( \varepsilon^e_{ij} \) is the elastic strain tensor; \( D_{ijkl} \) is the conventional linear elastic tangent stiffness tensor which can be expressed in term of shear (\( G \)) and bulk (\( K \)) modulus, \( D_{ijkl} = G(\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl}) + (K - (2G/3)) \delta_{ij} \delta_{kl} \) and \( \delta_{ij} \) is the Kronecker delta.

### 2.2. Calibration of the constitutive parameters

The constitutive law has been used to capture the response of Gravina calcarenite, a soft carbonate rock from Southern Italy that has been found to exhibit localized compaction [14,36]. The advantage of studying this material derives from the large number of triaxial compression experiments enabling the quantification of the model parameters [35,14], as well as from the availability of oedometric compression tests displaying global signatures of compaction banding [14,34,53]. As a result, this porous rock provides unique opportunities for theoretical/numerical studies focused on stress-path effects.

Although most parameters derive from a recent constitutive study by Buscarnera and Laverack [32] (Table 1), some material constants are here re-discussed in light of bifurcation analyses. Indeed, in presence of strain localization the post-localization regime is controlled by strain inhomogeneities, and constitutive analyses should be regarded only as approximations of the real sample response [55]. This aspect is crucial to calibrate the degradation parameter \( \xi_m \), which mimics inelastic phenomena in the brittle–ductile regime, where localized compaction is likely to occur. As noted by Buscarnera and Laverack [32], this model constant affects both the stress–strain response (Fig. 2b) and the domain of strain localization in the stress space (Fig. 2a). This property has allowed us to obtain a first-order estimate for \( \xi_m \), which has been evaluated by identifying the strain localization domain through the classical bifurcation condition by Rudnicki and Rice [39]:

\[
|A_{ijkl}| = |n_i L_{ijkl} n_j| \leq 0,
\]

where \( |A_{ijkl}| \) is the determinant of the so-called acoustic tensor. Condition (10) can also be used to define the orientation vector \( n_i \) of possible deformation bands, which have to be determined based on the characteristics of the fourth order tangent stiffness tensor \( L_{ijkl} \):

\[
L_{ijkl} = \frac{D_{ijkl} \partial g/\partial \sigma^p_{ij} \partial f/\partial \sigma_{mn}}{H + (\partial g/\partial \sigma^p_{ij} \partial p_{ijkl} \partial f/\partial \sigma^p_{ij})}
\]

### Table 1

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Definition</th>
<th>Calcarenite</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K ) (kPa)</td>
<td>Elastic bulk modulus</td>
<td>80,000</td>
</tr>
<tr>
<td>( C ) (kPa)</td>
<td>Elastic shear modulus</td>
<td>75,000</td>
</tr>
<tr>
<td>( \rho_m )</td>
<td>Parameter governing the volumetric degradation</td>
<td>4.5</td>
</tr>
<tr>
<td>( B_p )</td>
<td>Isotropic plastic compressibility</td>
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</tr>
<tr>
<td>( \mu_f )</td>
<td>Shape parameters of the yield surface</td>
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</tr>
<tr>
<td>( M_d )</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>0.9</td>
</tr>
<tr>
<td></td>
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<td>0.7</td>
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<td>( \rho_e )</td>
<td>Shape parameters of the plastic potential</td>
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</tr>
<tr>
<td>( a_t )</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>0.75</td>
</tr>
<tr>
<td>( M_s )</td>
<td></td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.67</td>
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<tr>
<td>( \xi_m )</td>
<td>Parameter governing the deviatoric degradation</td>
<td>0.75a</td>
</tr>
<tr>
<td>( R )</td>
<td>Size of the yield surface in the tensile stress domain</td>
<td>0.05c</td>
</tr>
<tr>
<td>( \rho_{el} ) (kPa)</td>
<td>Expansion in size of the elastic domain in cemented media</td>
<td>2200b</td>
</tr>
<tr>
<td>( \rho_{pl} ) (kPa)</td>
<td>Size of the initial elastic domain for cohesionless media</td>
<td>200b</td>
</tr>
<tr>
<td>( \alpha ) (s)</td>
<td>Viscosity parameter</td>
<td>131c</td>
</tr>
</tbody>
</table>

*a Initial assumption based on data from triaxial tests.
*b Initial values of the plastic internal variables.
*c Used only in finite element analyses to include rate-dependent regularization.
Fig. 2. Parametric study of the effect of the degradation parameter \( \xi_m \): (a) yield surface with localization domain; (b) simulated stress–strain response for triaxial compression.

Fig. 3. Localization analysis at different yield points (here function of the initial confining pressure prior to triaxial compression).

\[
H = - \left( \frac{\partial f}{\partial p} \right) \left[ 1 + r - \frac{\partial f}{\partial \varepsilon_n} \right] \left( \frac{\partial f}{\partial \mu} \right) \left( \frac{\partial f}{\partial \varepsilon_m} \right) \left( \frac{\partial f}{\partial \sigma} \right)
\]

(13)

By performing a parametric study it is possible to show the variation of the localization domain for different values of \( \xi_m \) (Fig. 2a). The domain is found to expand with increasing values of \( \xi_m \). Similarly, Fig. 2b indicates the variation of the predicted stress–strain response for varying \( \xi_m \) in two triaxial compression tests simulated at 1100 kPa and 2000 kPa confining pressure. It is apparent that the predicted constitutive response does not vary significantly with \( \xi_m \), while the extent of the bifurcation zone does. This confirms the convenient choice to assess such degradation parameter via the localization zone rather than through a direct comparison with the measured stress–strain behavior of the calcarenite.

2.3. Triaxial compression paths causing localized compaction

The simulations in Fig. 2 display a stress plateau, which can be associated with a pore collapse enhanced by structural degradation. As is typical for porous rocks sheared at high confinement, this stage is followed by a re-hardening trend [1]. Since these features of the stress–strain response are usually interpreted as indications of shear-enhanced compaction and/or pure compaction banding [15], it is convenient to assess the potential for strain localization along these paths. In the case of Gravina calcarenite, in fact, post-mortem observation of specimens sheared from an initial confinement of 2 MPa has disclosed the formation of pseudo-horizontal localization bands [14]. Similarly, a reinterpretation of earlier experiments performed by Lagioia and Nova [35] on the same rock has suggested the potential for formation of non-homogeneous shear-enhanced compaction in samples sheared at 1.1 MPa confinement [36].

The two stress paths in Fig. 2 can therefore be used to constrain the extent of the strain-localization zone and define a tentative value for the parameter \( \xi_m \). The analysis suggests that a value of 0.75 is sufficient to generate a localization zone large enough to encompass both paths. For this reason, \( \xi_m = 0.75 \) is used in Fig. 3 to define potential orientations of the deformation bands by plotting for different stress states the determinant of the normalized acoustic tensor against the band angle. Angles corresponding to zero or negative determinant suggest the possible formation of strain localization zones at the considered stress. Band orientations are expressed in terms of the angle between the normal to the plane of strain localization and the horizontal axis (Fig. 3). As a result, the stress domain associated with the potential formation of pure compaction bands is found to be located in the high-pressure portion of the yield locus, where horizontal bands (i.e., \( \alpha = 90^\circ \)) provide the minimum value of the acoustic tensor determinant. By contrast, at lower confinements, the inclination of the predicted localization zone changes, with high-angled shear bands becoming the preferential form of localization. To compare our analyses with previous results based on different conventions of stress invariants [3, 31, 56–58], we have computed a modified slope index for the yield surface \( (\mu = dq/d\sigma)/\sqrt{3}) \) and the plastic potential \( (p = dq/d\sigma)/\sqrt{3}) \). Both indices have been evaluated at the predicted onset of localization (see table inset in Fig. 3b), and the computed values are consistent with previous theoretical predictions [31], as well as with evidences of compaction banding and/or shear enhanced compaction available for various porous rocks [3].

This strategy can also be used to monitor the evolving potential for strain localization during deformation. This is shown in Fig. 4, in which the constitutive response predicted for the triaxial compression paths in Fig. 3 is analyzed. The localization analysis based on the bifurcation condition has been performed at several post-yielding states (open circle symbols in Fig. 4) by plotting the normalized determinant of the acoustic tensor against the band angle. As expected, both stress paths fulfill the bifurcation criterion at the onset of yielding, as the acoustic tensor determinant drops to zero or to negative values. Again, the formation of a shear-enhanced compaction band is suggested for the test simulated at lower confinement (1.1 MPa), while pure (horizontal) compaction bands are predicted for the stress path starting from a higher confinement level (2 MPa). It is interesting to note that the bifurcation indices tend to increase with further deformation, reflecting a reduced tendency of the material to undergo strain.
localization. This feature of the predicted response can be attributed to the evolution of the internal variable $p_m$ (Eq. (8)), which tends to decrease upon post-yielding shearing because of strain-softening. In other words, with decreasing values of $p_m$ the effects associated with the loss of structure tend to vanish, promoting a progressive re-hardening. These effects are controlled by the degradation parameters, and hence by $\xi_m$. As a result, the calibration of $\xi_m$ is found to exert an important control on the predicted patterns of localized compaction.

2.4. Effect of kinematic constraints: oedometric compression

As suggested by Buscarnera and Laverack [32], refinements of the calibration can be achieved by cross-correlating data from different loading paths. Oedometric tests, for example, can be a useful resource for compaction band analyses [38]. Indeed, the deformations associated with oedometric loading coincide with the kinematic conditions inside a compaction band. This idea is corroborated by data provided by Olsson [15] and Baud et al. [2], who report deviations of the measured strain path at the onset of compaction banding during triaxial compression tests performed at constant radial confinement. The authors reported indeed axial shortening taking place with negligible radial strains (i.e., a deformation mode enforced directly by oedometric tests). Along these lines, recent studies by Arroyo et al. [14] and Castellanza et al. [53] have indicated the occurrence of localized compaction during oedometric tests, showing that the onset of strain inhomogeneity was linked to specific global signatures (e.g., a peak of the vertical stress and/or a curl of the averaged stress path obtained from radial stress measurements). The $K_0$ consolidation response reported by Lagioia and Nova [14] for Gravina calcarenite displays similar features (see data reported in Fig. 11), thus suggesting that also this material is susceptible to localization processes upon radially constrained deformation. This evidence can be used to further constrain the value of the parameter $\xi_m$, thus obtaining a more accurate calibration of the model. This is shown in Fig. 5, which shows the stress paths and the associated localization analysis for two simulated oedometric compression tests characterized by different values of $\xi_m$. In the case of $\xi_m = 0.75$ (i.e., the value previously estimated from triaxial tests) the bifurcation analysis rules out localization processes, as the computed determinant is always positive (Fig. 5a and b). On the contrary, the use of $\xi_m = 4.0$ modifies the stress path (Fig. 5c and d) and increases the potential for mechanical instability [32].

This result can be explained with the fact that increasing values of $\xi_m$ cause the expansion of the localization domain (Fig. 2), thus favoring the intersection between the evolving zone of potential localization and the stress path [32]. This is confirmed by the inspection of the stress–strain response via bifurcation analyses, which provide negative values of the bifurcation indices (Fig. 5d). By inspecting the range of possible band angles, it can be noticed that inclinations of 90° are possible at a certain point of the deformation process (point iv). Despite this, horizontal bands are not the preferential localization mode, as inclined bands of shear compaction are activated first (at iii) and are featured by the lowest value of determinant even at strains for which the horizontal bands become theoretically possible. In other words, regardless of the value of $\xi_m$, the stress path generated by the oedometric constraint tends to cross the localization zone in a stress domain in which compactive shear bands are more likely to occur.

While these analyses highlight the interaction between kinematic constraints, stress path and localization mode [32,33], they cannot be considered to be conclusive, as the patterns of localized compaction in actual specimens eventually depend on material heterogeneity and boundary effects. This raises two major questions that will be addressed hereafter via numerical modeling: (i) is the adopted calibration procedure based on bifurcation analyses adequate to capture the global behavior of rock samples and the consequent localization patterns? And (ii) how do boundary constraints and material heterogeneity interact with the geometric patterns of localized compaction?

3. Finite element analysis of localized compaction

3.1. Regularization scheme

Reliable numerical modeling of strain localization in plastic solids requires regularization schemes to remove possible discretization dependent solutions [40,41,60,61]. Indeed, the energy dissipation during localization is controlled by the size of the
process zone. Given the lack of an internal length in traditional elasto-plastic models, such zone may depend on the mesh size [62], thus producing a pathological mesh dependency of simulations performed in the post-localization regime.

To overcome this problem, we have implemented a computationally inexpensive rate-dependent regularization of the Perzyna-type [63], which has been successfully used for several types of geomaterials [21,41,64,65]. The enhancement of the constitutive model has been carried out by modifying the plastic flow rule in the following manner:

\[ \dot{\epsilon}_p^R = \frac{\langle \phi(f) \rangle}{\eta} \frac{\partial \eta}{\partial \dot{\epsilon}_p} \]  

(14)

where \(\langle \ldots \rangle\) represents the McCauley brackets; \(\phi\) is the overstress function (here assumed to be given by \(f/(p_{y0} + (1 + r)p_{\text{min}})\); \(f\) is the current value of the yield function; \(\eta\) is the viscosity parameter and \(dt\) is the time increment during which an axial strain rate is imposed (\(\dot{\epsilon}_a = \frac{\partial \eta}{\partial \dot{\epsilon}_a}\)). A value of axial strain rate \(\epsilon_a = 10^{-6} / \text{s}\) has been used, as is typical for quasi-static loading. Moreover, the value of the viscosity parameter (\(\eta = 131 \text{ s}\)) has been chosen to obtain a rate-dependent response as close as possible to that of the rate-independent version of the model, while preserving at the same time the mesh independence of the computed solution.

Details about the calibration procedure of the selected regularization scheme can be found in [21].

The model has been implemented in the ABAQUS Finite Element code [66] through a UMAT subroutine. The constitutive relation has been integrated through an implicit algorithm, while the rate dependent regularization has been constructed through the algorithmic hierarchy proposed by Wang et al. [40]. The effectiveness of the regularization strategy has been assessed through a simple numerical exercise. Two plane strain simulations have been performed using rectangular specimens (40 mm x 20 mm) made with eight node quadrilateral finite elements and two mesh densities (800 and 2200 elements, respectively). The bottom boundary of the specimens has been subjected to roller boundary conditions, while the horizontal displacement at the bottom-left corner has been constrained to prevent lateral movements. Finally, both specimens have been subjected to roller boundary conditions, while the horizontal displacement at the bottom-left corner has been constrained to prevent lateral movements. Finally, both specimens have been subjected to a constant rate of displacement at the top boundary. The expected outcome from this numerical exercise is the activation of a shear band in specimens subjected to unconfined compression. To trigger the band, a slight weakness has been assigned at one of the bottom elements of each model (i.e. 1% reduction in \(p_{\text{min}}\) marked with a white box in Fig. 6a and b).

The effect of the mesh density is presented in Fig. 6, where the formation of a shear band is captured through the contours of...
plastic volumetric strain. At a certain value of axial strain both specimens form shear bands with identical features (i.e., the computed orientation, thickness and progression of the bands are identical). Most importantly the predicted axial stress–strain response (Fig. 6) is very similar, which ensures almost identical dissipation irrespective of the mesh size. The numerical test clearly indicates that the rate-dependent regularization scheme efficiently overcomes the pathological mesh dependency arising from bifurcation instability.

3.2. Finite element model of calcarenite specimens

The response of calcarenite samples has been simulated through 3D finite element models both for the case of triaxial compression and oedometric compression. For this purpose, two different types of specimen have been used. Triaxial tests have been simulated through a cylindrical specimen of size of 38 mm × 76 mm (Fig. 7a) discretized with 32 650 linear brick elements (8-nodes). Oedometer specimens have been assigned a size of 55 mm × 22 mm and discretized with 52 835 linear tetrahedron elements (4-nodes) (Fig. 7b). Vertical movements (Y) and rotations about the vertical axis have been prevented using appropriate restraints at the bottom boundary of each specimen. The horizontal (X-Z) movements of the bottom central node have also been restricted to avoid lateral instability. To ensure oedometric boundary conditions, additional constraints have been imposed in the oedometer specimen by restricting the radial displacements of the lateral boundary.

The loading process has been applied in two steps; (a) initially both specimens have been subjected to isotropic compression ($p_0$); and then (b) displacement control ($\varepsilon_a = 10^{-6}$) has been applied at the top boundary. All the parameters for calcarenite given in Table 1 have been used, except $\xi_m$ which has been assumed to be equal to 4.0, as indicated by bifurcation studies. To initiate heterogeneous deformation, a stress concentration is needed to create a hotspot of inelastic restructuration. This aspect has been included in the model through a simulated material heterogeneity (Fig. 7), here imposed via random spatial variation of $p_{\text{mo}}$ with ± 1% from the average calibrated value and standard deviation of 0.014. This strategy generates varying yielding points at different locations within the specimen, thus allowing the spontaneous generation of heterogeneous compaction zones.

3.3. Simulation of specimen response upon drained triaxial compression

Drained triaxial compression has been simulated to track formation and propagation of compaction zones, as well as to reproduce the global response of calcarenite specimens. To locate the areas of the samples subjected to concentrated inelasticity and loss of strength, the variation of second-order work has also been monitored. The first simulation is a compression test starting from a hydrostatic confinement of 2 MPa, i.e. a condition that in experiments has originated heterogeneous deformations in the form of horizontal compaction zones [14]. Fig. 8 reports the contours of cumulative and incremental plastic volumetric strains in the simulated sample, as well as the local second-order work at different stages of the process (open circles in Fig. 9). Compaction bands are mostly accumulated at the boundaries (see $\varepsilon_a = 0.008–0.016$ in Fig. 8) and propagate towards the center of the specimen. Two mechanisms of band development are found: (i) bands that derive from stress concentration and extend across the width of the specimen and (ii) progressive formation of new bands aligned at different locations along the axis of the specimen. Negative values of computed second-order work are concentrated inside the bands, thus defining the active zone of inelastic strain localization. By contrast, positive values are found outside the bands, within portions of the sample undergoing elastic unloading. As discussed with reference to material point analyses, the potential for strain localization decreases once the mechanical degradation stage is complete, with densely packed conditions causing the re-hardening of the specimen. Once these conditions are attained, a homogeneous response is restored in the strain-hardening regime (Fig. 8).

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**Fig. 7.** Finite element mesh for (a) triaxial compression tests; (b) oedometer tests with random spatial heterogeneity in numerical specimens of Gravina calcarenite.
The computed solution clearly supports the predictions obtained through material point simulations, as indeed the band inclination coincides with that derived from a localization analysis (Fig. 4) corresponding to the minimum acoustic tensor determinant. As discussed by Das et al. [21], this feature can be seen as an outcome of the maximum dissipation principle in the localization plane, according to which the band inclination associated with the minimum value of determinant of the acoustic tensor can be seen as the natural weakest direction of deformation.

Fig. 8. Simulated distribution and propagation of compaction bands in triaxial compression tests (2000 kPa initial confinement) on Gravina calcarenite specimen.

Fig. 9. Stress–strain response for simulated triaxial compression tests at 2000 kPa initial confinement. A comparison with measured data is reported (data after [35]).
The accuracy of these simulations can also be assessed by comparing the simulated global response with measured data for calcarenite specimens. This comparison is provided in Fig. 9 in terms of both stress–strain behavior and volumetric response. The figure illustrates a satisfactory agreement between computations and experiments, thus corroborating the accuracy of our calibration strategy.

4. Simulation of the effect of boundary constraints

Triaxial compression produces highly controlled stress paths that cross the bifurcation domain in predefined locations. This feature is likely not to reflect conditions in the field, where the stress path results from local burial history and complex tectonic processes [33]. Oedometric tests can therefore be a useful scheme to study realistic features of compaction banding [38], as they mimic a simple deposition history (i.e., $K_0$ consolidation) and impose boundary constraints able to generate the same strain kinematics taking place in pure compaction bands. Gravina calcarenite offers an interesting opportunity to meet this goal, as its $K_0$-compression obtained from triaxial testing exhibits considerable loss of structure and pore collapse. Although the original calcarenite samples tested by Lagioia and Nova [35] were discarded without subjecting them to post-mortem inspection, subsequent studies by Arroyo et al. [14] and Castellanza et al. [53] on similar materials have reported horizontal compaction zones. Most of these studies were based on a modified oedometer with deformable boundaries, which was able to produce a stress–strain response similar to that observed in $K_0$-compression tests done in a triaxial cell [34,35]. For this reason, we have reproduced numerically the conditions imposed in both types of experiments, with the aim to elucidate the processes that may have originated localized compaction in the tested samples.

4.1. Rigid boundary constraints

To compare numerical predictions and measured data, a finite element model of a slender specimen (Fig. 7a and b) has been used to mimic the $K_0$-consolidation originally performed in a triaxial cell (where average radial strains were prevented through an automated servo-control, [35]). In this case, the $K_0$ stress path has been replicated by applying varying horizontal nodal forces at the lateral boundary. The values of such varying radial stresses required to prevent average lateral strains have been inferred from a prior material point analysis. Moreover, to understand the mechanisms that may have caused localized compaction in oedometer tests done in subsequent studies [53], a second numerical model has been used, which is closer to the sample geometry used in a typical oedometer apparatus (Fig. 7c and d). In this case, the experiment has been simulated in a simpler way, i.e. by fixing the horizontal displacements of the lateral boundary, thus directly preventing the occurrence of radial strains. To replicate the same initial conditions of the experiment, both models have been hydrostatically compressed up to a pressure of 210 kPa and then deformed axially by imposing the vertical displacements at the top boundary. Fig. 10 shows the computed deformation patterns in the numerical specimens, showing that in both cases shear zones develop inside the domain.
Positive plastic volumetric strains within the band highlight the compactive nature of the localized process. Despite horizontal bands may be seen as a natural mode of strain localization for this type of loading, the analysis shows that the stress path generated by the imposed constraints induces localized shear zones inside the specimen. While such non-trivial mechanisms do not match the symmetry imposed by the boundary conditions (especially in the case with rigid lateral constraints), the possibility of activating a shear zone was already predicted by the bifurcation analysis in Section 2. In other words, the complex deformation pattern in Fig. 10 can be interpreted as the spontaneous outcome of local stress paths that cross the bifurcation domain in the zone of compactive shear bands rather than in correspondence of the domain of pure compaction banding.

Fig. 11 superposes the computed global behavior with the data for $K_0$ consolidation reported by Lagioia and Nova [35]. Although the three curves can be compared only qualitatively, it is readily apparent that their stress paths share similar attributes. On the one hand, such result confirms the interpretation of earlier experiments [14], in which these attributes were interpreted as a signature of strain localization. On the other one, they point out that the interpretation of these global signatures as pure horizontal compaction bands might be misleading, as it can overlook complex localization processes that are not easily detectable through boundary measurements.

4.2. Flexible boundary constraints

A factor of interest for the onset of localized compaction during constrained deformation is the flexibility of the boundaries that impose the kinematic restraints. While the use of rigid boundaries is typical for oedometer testing, flexible boundaries can be adopted to measure the radial stress originated by a constrained deformation. This configuration was adopted by Arroyo et al. [14] and Castellanza et al. [53] in the apparatus used to detect horizontal compaction bands in specimens of highly porous geomaterials.

To simulate such conditions, the numerical model has been enriched by adding a flexible ring around the specimen. Brass was used to simulate the ring ($G = 37.59$ GPa and $K = 100$ GPa), which was eventually discretized via the same finite elements used for the calcarenite sample. Given the deformability of the lateral boundaries, the specimen is allowed to slightly expand during vertical compression. The compressive load has been applied using a displacement boundary condition for the rigid plate on the top of the specimen, while a second rigid plate has been placed at the base of the specimen to restrict vertical movements. Steel has been used to simulate the top and bottom plates ($G = 78.74$ GPa and $K = 144.9$ GPa), with the purpose to create sufficiently rigid boundaries, and a small friction coefficient of 0.1 has been imposed at the interface between the specimen and the rigid boundaries. This arrangement is sketched in Fig. 12a, and has been used in combination with a calcarenite model identical to the specimen shown in Fig. 7 (i.e., again characterized by a random spatial heterogeneity).

Fig. 12b shows the computed patterns of deformation in terms of cumulative and incremental plastic volumetric strains. It can be readily observed that flexible lateral boundaries and small amounts of friction promote the formation of horizontal compaction bands. These bands are originated at the top and bottom of the specimen and propagate towards the center, thus reproducing a response very similar to that observed in the previously mentioned experimental studies. In addition, the simulations show that minor alterations to the boundary

![Fig. 11](image1.png)

**Fig. 11.** Comparison between computed response and measured data for oedometric compression of Gravina calcarenite; (a) stress–strain response; (b) stress path (data after [35]).

![Fig. 12](image2.png)

**Fig. 12.** Numerical simulation of $K_0$ consolidation with flexible ring oedometer, showing the propagation of compaction bands.
conditions are sufficient to alter the localization response, thus considerably deviating from the idealized conclusions obtained from a bifurcation analysis of the constitutive predictions.

4.3. Effect of patterned material heterogeneity

Here we study the role of the spatial pattern of heterogeneity, passing from a random distribution of the internal variable controlling the yielding threshold \( (p_m) \) to a layered heterogeneity. In other words, a spatially varying \( p_m \) has been assigned along the vertical axis \( (Y) \), while the material parameters have been assumed to be homogeneous across horizontal planes \( (X-Z) \), as shown in Fig. 13. This scheme mimics the natural heterogeneity of sedimentary formations, in which depositional layers of lithified material form under high pressures, creating patterns of spatially varying density and strength. Similar to kinematic conditions, such geometric features constrain the mechanical response and may force the system to deform in accordance with the symmetry requirements. As a result, it is argued that a spatially patterned structure may influence also the formation of compaction bands in layered rock masses, as it has been found both in field and laboratory investigations by Aydin and Ahmadov [67] and Townend et al. [68], respectively.

Once a vertical layering has been assigned, the localization process is initiated at the weakest zone, affecting the entire layer that has reached yielding conditions. This process generates horizontal compaction bands that propagate towards the boundary of the specimen with further deformation. At variance with the previous cases, no lateral extension of these bands is obtained, as each band forms across an entire layer. In addition, as a result of boundary effects the band alignment tends to change as the localization process approaches the top boundary of the specimens.

Fig. 14 compares the stress--strain response and the stress path associated with the three numerical simulations of oedometer samples. As is readily apparent, the macroscopic averaging of the external quantities generates global responses that are not easily distinguishable one from another, thus indicating that such heterogeneous deformation mechanisms generated by oedometric compression (e.g., non-symmetric shear zones or pure compaction bands) are associated with similar macroscopic signatures, and are therefore not easily distinguishable via external force–displacement measurements.

These results (Fig. 14) prompted additional inspections of the local response within the localization zone, with the goal to elucidate the mechanisms underlying the patterns of localized compaction predicted in the oedometer simulations. Local stress paths at three selected integration points (marked with a white triangle in Fig. 15a, d, g) have been plotted in Fig. 15(b, e, h). All the selected points are located inside the process zone of heterogeneous compaction, thus providing a snapshot of the active deformation mechanisms inside the bands. Furthermore, localization analyses similar to those discussed in Section 2.4 have been used to track the characteristics of the localization events at specific stress states along the computed paths (states i and ii). Such analyses have been performed in a qualitative manner, by exploiting the similarity between the response provided by rate-independent and rate-dependent formulations (as indeed the latter cannot be rigorously analyzed via the localization condition in Eq. (11)). In other words, rate-independent localization analyses have been carried out for stress states very close to those computed through the regularized finite element model. For this purpose, the elasto-plastic constitutive tensor was re-computed by

![Fig. 13. Numerical simulation of \( K_0 \) consolidation in calcarenite specimen with pattern heterogeneity, showing the propagation of compaction bands.](image)

![Fig. 14. Comparison of the response computed for the three simulated oedometer specimens.](image)
using the same hardening parameters \((p_s, p_m)\) and modified stress-ratios \(\eta^* = q/(p + r.p_m)\) obtained from the numerical simulations at the selected points. This strategy has allowed us to quantify the localization potential, thus identifying the preferential localization modes at the selected points and providing a mechanistic interpretation for the predicted patterns of heterogeneous compaction.

Fig. 15 displays the evolution of the normalized acoustic tensor at the three selected points. In all cases the discontinuous bifurcation is predicted to be initiated in the form of an inclined shear band, eventually turning into pure compaction localization with horizontal band angles. Nevertheless, Fig. 15b indicates that the simulation characterized by rigid boundaries and random heterogeneity deviates significantly from the ideal stress path associated with oedometric conditions (Fig. 5c). In addition, stresses prone to pure compaction banding are achieved only when the values of the acoustic tensor determinant computed for \(\alpha = 90^\circ\) are just below zero (i.e., there is no longer significant potential for localization when a horizontal band becomes the preferential mode of heterogeneous compaction, Fig. 15c). Such characteristics are clearly an outcome of the prior shear band mechanism, which deteriorates the potential for further strain localization and reduces dramatically the likelihood of pure compaction banding right at the beginning of the stage of inelastic loading (Fig. 10). By contrast, the use of flexible boundary constraints and layered heterogeneity tends to promote local stress paths that maintain a significant potential for pure compaction banding up to stress states located in proximity of the plastic cap (Fig. 15e, h), thus favoring the formation and propagation of horizontal compaction bands (Fig. 15f, i).

5. Conclusions

We have studied the patterns of localized compaction emerging from constrained and unconstrained axisymmetric loading on simulated specimens of porous calcarenite. In the first part of the paper we have discussed a strategy to refine the calibration of the model parameters by means of the bifurcation theory. It has been shown that the cross-correlation of data from different stress paths can be used to quantify material properties and achieve improved predictions. In addition, the dependence of strain localization on the confinement stress has been captured correctly, reproducing transitions from high-angle shear bands to pure (horizontal) compaction bands.

In the second part of the paper, finite element analyses have been used to investigate the role of loading paths and kinematic constraints. Rate-dependent regularization and spatial randomization of the rock properties have allowed us to reproduce realistically the response of calcarenite specimens, obtaining a satisfactory agreement with the measured data. Such numerical model has been used to inspect the effect of heterogeneity and boundary effects on oedometric compression, a loading mode useful to understand the mechanics of compaction in the natural environment. It has been shown that certain types of boundary conditions (e.g., flexible lateral boundaries with friction) tend to divert the stress paths towards the domain of pure compaction banding, while other conditions (e.g., rigid lateral boundaries) exacerbate the tendency to develop shear zones. In all cases, however, the development of heterogeneous deformation zones has been predicted to disappear with increasing strains. In addition, the averaging of the quantities computed at the boundaries has been
found to generate global signatures that are not easily distinguishable from those of pure compaction banding, suggesting that the identification of specific patterns of localization from force-displacement measurements can be particularly elusive if not complemented by local measurements at selected stress/strain levels.

The numerical results reported in this work provide guidance to identify compaction bands at both laboratory and field scale, especially in case of unconventional stress paths mimicking the effect of natural processes. In particular, they disclose two major features of localized compaction: (i) the structures generated by these mechanisms tend to disappear upon further straining, and (ii) their geometric and mechanical characteristics may not be necessarily regarded as a pure product of the constitutive response of the parent rock, but rather as the outcome of complex interactions between structural effects, boundary conditions, local heterogeneities and material properties. These findings may provide a justification for the elusive characteristics of pure compaction bands, which until now have been found in the field only under very particular circumstances.

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