Discrete micro-physics interactions determine fracture apertures

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Abstract An important question arises in relation to a rock-mass that is disrupted by an array of fractures, namely: how to quantify the evolving spatial arrangement of fracture apertures that are a major factor in bulk fluid flow processes. The approach herein employs a discrete micro-physics model of the rock texture, enabling the formulation of analytical expressions that explicitly define the fluids/geomechanics interactions that occur at the micro-scale. The resulting macro-scale responses of the model define the stress, bulk strain, and pressure states that characterise the porous rock. Via extending the discrete model by introducing a planar discontinuity, the fracture-normal bulk strain determines the status of the fracture aperture, as a consequence of the movement of the rock/fracture interface. The micro-physics model shows that a closed fracture cannot change to an open fracture by pressure changes alone; instead, bulk strain must elongate the porous rock in a direction normal to the fracture. Once opened, fracture apertures respond to changes in fluid pressure. A realistic context, within which the required bulk strain occurs, is the discontinuum geomechanics of fractured rock-mass systems, for which previous simulations exhibit a range of emergent local states that relate to the conditions, identified via the micro-physics, as being the essential controls on aperture evolution.

Article highlights

- Discrete rock-texture model underpins micro-physics expressions that lead to macro-scale material response of matrix/fracture
- Closed fracture cannot open without local elongation normal to fracture; high pressure alone does not open fracture
- Open fracture changes aperture with changing pressure

Keywords Fracture aperture · Micro-physics · Micro-to-macro · Fluid–solid interaction · Effective stress

1 Introduction

A rock fracture is defined here as a macro-scale deformation feature, normally expressed as a quasi-planar geometric entity, which disrupts the prior connectivity of some volume of rock. The length-scale of a fracture is much larger than the length of the characteristic textural elements of the rock, such as the grain size. The creation of a new fracture is sensibly related to an evolving physical state that owes its evolution to
some set of processes – such as changing bulk strain, changes of temperature, alterations of local fluid pressure, etc. While there may exist either esoteric or practical reasons to be interested in identifying the events that led up to the formation of a fracture, a utilitarian approach can set those considerations aside. In such a ‘performance’ perspective, it is possible to focus only on the role of the fracture in the alteration of some process that occurs later in geological time, such as that associated with human interventions in the subsurface, with an important example being fluid extraction from a fractured reservoir (Spence et al. 2014).

This paper is framed in the ‘performance’ category, and the attention here is restricted to an examination of what physical conditions cause a pre-existing fracture to experience opening or closing of its void space. Fluid pressure is an important physical condition that exists within the pore system of the wall-rocks adjacent to the fracture, and within an open fracture. The analysis here is restricted to the case where the pore pressures in the rock (the ‘matrix’) and within the (open) fracture are equal, but the approach can easily be extended to the case where the two pressures differ. The fracture itself does not possess a state of stress, since the notion of stress is associated with solids. In the case of a closed fracture, a compressive normal stress can exist, as well as a shear stress, on the plane of the fracture. It is important to appreciate that these stress components exist within the matrix rock that exists on either side of the fracture, and the inference of their presence on the fracture plane is via resolving the matrix state onto an imaginary internal plane oriented in the fracture orientation. Thus, the question of stress state conditions ‘on’ the fracture plane actually is a matter of determining the stress state within the adjacent matrix. That is the central focus of this paper.

The interplay between fluid pressure and stress state has long been recognised as important in the case of porous materials, and especially for geomaterials. The notion of effective stress emerged in the early 20th Century through the experimental work of Fillunger (1913) and Terzaghi (1923), as a useful laboratory parameter. The idea was subsequently elevated into being a constitutive law (Fillunger 1936; Terzaghi 1936), in the form widely recognised today as the law of effective stress. Biot (1941) developed a micro-physics perspective of effective stress, within which he separated the solid skeleton and the pore elements, allowing a consideration of the state (pressure and stress) interactions at the interfaces between solid and fluid.

In Biot’s theory, he imagined that the solid has a uniform state of stress. This follows from the perspective that a porous rock is a solid material punctuated by isolated and non-interacting, fluid-filled voids. Ideas from the world of ‘digital rocks’ – a topic that has matured over the past two decades (Bakke and Øren 1997; Blunt et al. 2012; Andrä et al. 2013; Bultrueys et al. 2016; Jiang et al. 2018; Zhao et al. 2019) – imagine a porous-rock model in terms of a pore system that can be depicted as a multi-connected network. It follows that the solid skeleton is also a multi-connected network (Fig. 1). Together, these

![Fig. 1 Example of the extraction of the pore network and the skeleton network from a digital-rock model. Left image shows a 3D grey-scale model, with solid depicted in grey and pore in black, derived via x-ray tomography, in this case using a sandstone. The middle image is the pore network extracted from that digital-rock model, using the method described in Jiang et al. (2007). The right image shows the network model of the solid skeleton, acquired via a method based on the one used in the extraction of pore networks In these networks, the bonds are shown in red colour, and the nodes are in green, scaled to the physical size of the elements in the digital-rock model](image-url)
perspectives point towards a discrete model for a rock matrix that depicts the solid skeleton and pore system as two space-filling, complementary objects that each possess a geometry and topology.

From this modern perspective of porous geomaterials, a discrete approach to poromechanics, comparable to Biot’s pioneering work, has been emerging. In this discrete micro-physics approach, it is recognised that the solid skeleton does not have a uniform state of stress (Ahmad et al. 2019). Of particular importance, the interactions between pore fluids and solid elements are understood to cause movement of the pore/solid interfaces (Müller and Sahay 2017) – a component of the system work which Biot ignored. There are multiple factors that distinguish these modern views in comparison with the simple model adopted by Biot and those who have followed along that path.

A simplification of the solid and pore networks, into regular 3D lattices, allows the derivation of closed-form analytical expressions that define the macro-scale responses of the porous material due to changes in mechanical state and fluid pressure (Couples 2019). This model is employed here as the means to link the micro-scale and macro-scale, in the context where there is a pre-existing planar fracture. This paper addresses the macro-scale state changes that are necessary to allow closed fractures to open, and what conditions govern the subsequent evolution of the fracture opening (or its aperture). The approach relies on bulk strains to link the micro//macro scales, and assumes that far-field (or boundary) tractions for the micro-scale are equivalent to the stress state of the macro-scale. Of course, pressure has the same meaning in both scales. An key point is that it is the bulk strains, in the case of a fracture-bounded matrix block, that determine the movement of the bounding face of the matrix model, and thus the displacement of the fracture wall.

The micro-physics analysis has been used in earlier work to develop process understanding in relation to the formation of mineral veins (Couples 2021a), as well as in an assessment of the validity of the enriched-continuum paradigm (Couples 2021b). A simpler analysis of the topic of the current paper was presented in Couples (2020; 2021c). Recent work is comparing the analytical model’s predictions against experimental observations of the Biot coefficient (Müller et al 2022). These investigations focus on the issue of pore boundary deformations (Müller and Sahay, 2013; 2016a, b; 2017), and the related implications for the system energy budget (linked to the consequential virtual work terms, which are missing in the Biot formulation). The current paper focuses on a deeper development of the micro-physics understanding that underpins the behaviours of the rock//fracture interface.

The paper is organised as follows. The next Section examines the relationships of the micro-physics understanding to the macro-scale setting of a matrix block bounded by a fracture plane, and identifies a sequence of loading steps and associated state changes that are necessary to transform a closed fracture to an open one. It includes a brief summary of the basis of the analytical micro-physics model, whose detailed derivation has been presented elsewhere. The specific set of conditions suited to the paper’s purpose are employed (explained in the Appendix) to derive a general expression that links the bulk strain in the fracture-normal direction, with the roles of the principal stress in that direction, and the fluid pressure. The subsequent Section focuses on the central point of the paper, which is that it is the responses of the matrix rocks around a fracture which govern the closed//open state of the fracture. The text describes a sequence of loading steps that lead to the transition of a closed fracture to its opening and enlargement of the fracture aperture. The Discussion Section consists of five sub-sections. The first assesses the similarities and differences between the micro-scale model and the commonly-adopted continuum-based models. The next sub-section examines the idea of effective stress, with a focus on the unhelpful perspective on stress states that is the consequence of reliance on process explanations based on effective stress. The third sub-section is a brief outline of the complex stress states that emerge in discontinuum geomechanics models of multi-fractured rock-mass systems, and emphasises how such systems provide the macro-scale circumstances for fracture aperture opening and evolution, as identified by the micro-scale method. The fourth sub-section considers the extension of the micro-scale understanding to the case of fractures that are ‘imperfect’, and whose characteristics are not as simple as the idealised arrangement adopted in the micro-physics formulation. A final
sub-section looks at the perspectives for further application of the micro-physics approach.

2 Macro-scale//micro-scale inter-relationships

A change in the aperture of a fracture – this is a macro-scale phenomenon – is precisely the consequence of differential displacements of the bounding walls of the two matrix blocks that meet along the fracture plane. In order to elucidate the geometric changes (which depend on the bulk strains, and the constraints assumed) that govern the movements of the walls of fractured matrix blocks, it is useful to refer to a simple configuration as a basic case (Fig. 2). To focus on the central issues, the case is illustrated as a series of equal-sized matrix blocks, arranged side-by-side along the x-direction (which is the fracture-normal direction; Fig. 3), with the faces of the discrete blocks initially touching (i.e. infinitesimal fracture apertures) in the reference configuration (middle of Fig. 2). The block-bounding fracture surfaces are oriented in the y–z plane, and in the middle of each matrix block in Fig. 2, there is a marker (shown as a dashed line) oriented parallel to the fractures, also in the y–z plane.

For any two adjacent blocks of matrix, their reference surfaces might remain fixed relative to external coordinates (lower set in Fig. 2), which equates to no bulk strain in the x-direction ($\Delta \bar{\varepsilon}_x = 0$, where bulk strain is indicated by the overbar). In this bulk constraint, a volumetric shrinkage (here expressed as contraction in the x-direction only) is needed to allow the fractures to open. An alternate possibility is that the reference surfaces experience relative movement, and thus there is macro-scale strain. If the reference markers move apart (top set of Fig. 2), so that $\Delta \varepsilon_x < 0$ (where compressive strain figured as positive), the matrix blocks undergo unloading and thus a reduction of the fracture-normal stress. If that process leads to complete unloading, the fracture surfaces can then open. The importance of this point – the requirement for reduction of normal stress – is based on the

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Fig. 2 Cartoon illustrating the two possibilities by which previously-closed fractures, separating equal-sized individual matrix blocks arranged in a series, may become open. (Centre) Reference configuration, with fractures closed. Dashed vertical line is the centerline of each block. (Top) Shows the case where blocks are moved apart by an unspecified bulk strain process, allowing fractures to open (after unloading blocks, see text). (Bottom) Shows the case where the individual blocks shrink in dimension by unspecified process (example process discussed later in text)
The detailed formulation of the micro-scale model is presented in Couples (2019). The role of the micro-scale model is to develop the macro-scale response due to changes in pore pressure and mechanical loading. In this sense, the micro-scale model defines the behaviour of a ‘material point’ as a function of macro-scale conditions of state. The role of thermal changes can also be addressed via the model, but those are not considered in this paper. Aspects of the macro-scale implications of this micro-scale model (i.e. the resulting behaviour of a material point) have been addressed in subsequent papers. Some of its ramifications for the Biot theory of poroelasticity are reported in Couples (2021a, 2021d) and in Müller et al (2022).

Application of the model in situations with discontinuities has been the principal subject matter in conference papers by Couples (2020, 2021b, 2021c), and the present paper is a more rigorous treatment of this use.

A derivation of the expressions that define the micro-scale model is presented in the Appendix, with a focus on the equations needed for the specific
situation addressed in this paper – the case with a pre-existing discontinuity. Although the model is fully defined by a set of mathematical expressions, it has proven useful to associate the form of those expressions with a geometric depiction (Fig. 4). A lattice is created by repetition of a unit cell in three directions; here the coordinates are orthogonal. The junction and the rods of the unit cell are all imagined as individual rectilinear hexahedral elements. This is a choice that permits the model expressions to be formulated in Cartesian coordinates without the un-necessary mathematical complexity demanded if the image were to be chosen to involve curved surfaces. The square-section rods are defined by their axis direction, which is the direction of the normal to the plane of intersection of the junction and the rod.

In this continuous model created by replicating the unit cell, the wetted faces — where the fluid pressure acts — are only the lateral faces of the rods (i.e. the rod faces whose normals are NOT the axis direction for that rod). All faces of each junction are covered by the adjacent rods, and so they are not wetted. It is imagined that bounding planes pass through the sets of rods that cross the model’s boundaries, midway along the rod lengths. These ‘planes’, composed of an array of cut segments of rod elements, create the locations where the mechanical boundary conditions of the model are imposed. In the configuration suited to the aim of this paper, one of these boundary planes is taken to be the fracture plane. If two such models, with ‘fracture’ planes, are placed adjacent, with the cut faces touching, the regularity of the lattice continues. If the model responds to loads, under the given constraints, in such a way as to cause the cut faces to separate, that is taken to be a macro-scale fracture-opening event.

Via the derivation given in the Appendix, in which the fracture-parallel bulk strains are not allowed to change (e.g. $\Delta \varepsilon_y = \Delta \varepsilon_z \equiv 0$), the applicable micro-scale model expression (Eq. 21) for the matrix material point is:

$$
\Delta \varepsilon_x = \frac{1}{E} \left[ \Delta \sigma_x \left( \frac{1 - v + tv - 2v^2 + 4nv^2 + 2r^2v^2}{(1 - v + tv)} \right) - \Delta P \left( \frac{2tv + 2nv^2 - 2r^2v^2}{(1 - v + tv)} \right) \right]
$$

(1)

This expression of the model indicates that the matrix will elongate in the x-direction if the pressure is increased while the x-direction stress is unchanged. Alternatively, if the pressure is unchanged, there is a linear relationship between the change in x-direction stress and the x-direction bulk strain. Most importantly, if the circumstance prevents a change in x-direction strain, a pressure increase causes an increase in the x-direction normal stress (and in the other stress components also). In ALL situations where there is a pressure change (whether an increase or decrease), the familiar and expected (from continuum-based material laws) linearity in the bulk strain and normal stress relationship is not found. The manner by which the role of pressure is expressed is different to the assumption often made when invoking the law of effective stress, and this point is directly addressed later in the paper.

Following on from the discussion around Fig. 2, there is value in discussing the boundary conditions adopted in the formulation of Eq. (1). In the x-direction, consider first the case where $\Delta \varepsilon_x = 0$. This bulk constraint means that the matrix does not experience a change in the total x-direction length of the (arbitrarily-sized) matrix block. This condition is probably appropriate for a simple setting of continuous rock that is not experiencing long-term and ongoing tectonic deformation, nor any other changes to its skeleton (such as diagenesis). It could also be suitable for many short-term processes that occur within a reservoir volume, even though that volume of rock may be subject to thermal and hydraulic perturbations. The basis of this assertion is as follows: a given volume of rock is surrounded by other rock volumes, which, in the naïve perspective of an infinite continuum, are experiencing identical condition changes. Thus, any putative lateral movement of the boundary or limit of one block/volume cannot occur without a compensating movement of the boundaries of the adjacent blocks. The assumed constraint that suppresses movement of the block boundary is appropriately described as a no-strain condition, and this may be an appropriate default choice for simple situations. However, via the analysis described in the following Section, the existence of open fractures demands that situations within a rock-mass must occur such that this default assumption is no longer the appropriate constraint.

It is similarly useful to comment on the selection of the assumed boundary conditions in the fracture-parallel directions, which here are assigned as no-strain changes in both the y- and z-directions.
The circumstances of interest here concern the macro-scale state changes that are necessary to allow a closed fracture to become, and then remain, open —possibly with further changes of aperture — or to experience a reduction of aperture, or even close after already being open. Each of these status transitions is the result of macro-scale state changes that cause some ‘critical’ condition to be reached, such that the evolution of the system subsequently occurs in circumstances of different constraints, new relationships, etc. The state changes identified are explained below. A catalog of the processes leading to such critical conditions, defining a rational sequence of evolution, leads to the idea of a set of process steps. To understand the poromechanical aspects of that evolution, it is convenient to describe the changes of macro-scale mechanical aspects as a sequence of loading steps. Here, the loading steps are expressed via analytical expressions that quantify the bulk responses of the micro-scale model to the macro-scale condition changes needed to reach the critical conditions for the transitions of the fracture status. The micro-scale model cannot explain the ultimate origin of the non-local events that are implied by the sequence. However, some exemplar settings, which provide illustrations of fracture responses that occur within a broader context, are described later in the paper.

In the micro-scale model, and when the fracture is closed, the configuration of the lattice (Fig. 4) is effectively undisturbed at the fracture plane, with no change of the textural characteristics at the (closed) fracture plane. If (or when) the fracture opens, the now-isolated micro-physics model, which conceptually sits on one side of the fracture (Fig. 3), is employed, via appropriate boundary conditions, to determine the bulk response of a matrix block that is bounded by a fracture plane. When there is an open fracture, the original position of the discontinuity plane serves as the reference location for quantifying the magnitude of the displacement of the wall of the matrix block (which is half of the aperture change, since the opening is assumed to be symmetric about that plane).

A few comments are warranted before the loading steps are presented in sequence. These address some points of possible confusion that can arise when employing macro-scale ideas at the micro-scale.
While in the closed condition, a compressive stress $\sigma_x$ normally exists on the discontinuous faces of the truncated rod elements (Fig. 4), representing a continuity of state from one matrix model to the adjacent matrix model, across the fracture plane. As long as a positive normal stress exists on the fracture plane, this indicates that there is elastic potential energy in the adjacent matrix blocks (Eq. 2). While in contact along the fracture, the adjacent blocks, with identical elastic states (and properties) are in equilibrium, and the interface between the blocks does not translate. If the elastic potential energy states somehow were to become unequal across the fracture plane, then the wall of both blocks will move until a new state of equilibrium is established. The potential energy change in one block is translated into physical work, with that work causing changes in the potential energy of the adjacent block. Such a change of equilibrium position of the interface (and thus changes of state in the matrix block) is described in the loading sequence below, especially in relation to the state changes associated with the transition from a closed fracture to an open one (loading step 3).

The concept of potential energy and its relationship to movement of the block boundary is important in understanding the changes of conditions necessary to allow the fracture to experience a transition, from the closed state, to being open. Consider first a micro-scale model that is ‘dry’ (no pore-filling fluid). Imagine that the present physical state is one where a compressive normal stress exists ($\sigma_x > 0$). Now, imagine that a virtual (infinitesimal) gap appears along the fracture plane — this means along the truncated rod-to-rod interfaces. Since there is no ‘material’ in the virtual opening, the notional gap represents a region of lower (minimum of zero, if the virtual space is in a vacuum condition) elastic potential energy. Therefore, the lattice model expands in the $x$-direction ($\Delta \varepsilon_x < 0$), lowering the magnitude of elastic potential energy within the skeleton (if there are no other changes). The existence of compressive stress means that there is potential energy to cause the block to expand against a region of lower potential energy. Thus, the fracture cannot become open while a positive normal stress exists on the fracture-plane. In the following analysis, the range of circumstances necessary, to diminish the normal stress on the fracture, are captured by adoption of the step-change boundary condition $\Delta \varepsilon_x < 0$.

It is important to emphasise that the notion of effective stress (a continuum construct) does not have a role in the solution of the micro-scale material response, which involves a model that explicitly depicts the solid skeleton and the (fluid-filled) void space. At the micro-scale, the idea of effective stress has no meaning, and thus does not exist. From a set of physical conditions (stress components and pressure), calculated via the micro-scale model, it is possible to calculate the macro-scale state of effective stress, since this is simply (and only) an algebraic operation that determines the difference between the set of (apparent) boundary stresses, and the fluid pressure. It is important to emphasise that it is inappropriate to assert that a rule or concept, which is based on macro-scale rules about the role of effective stress, is applicable at the discrete micro-scale. This point is examined further later in the paper.

Starting with a pre-existing and still-closed fracture (this is exactly equivalent to a no-strain micro-physics case without a fracture), and assuming that fracture-normal bulk strain is inhibited ($\Delta \varepsilon_x = 0$), Eq. (1) shows that an increase of pressure alone always increases $\sigma_x$, so $\Delta \sigma_x > 0$ in the circumstance of increasing pressure $\Delta P > 0$ (Fig. 5). Because of reversibility in this model, a reduction of pressure leads to a reduction of stress.

The relationship between pressure and stress stems from the fact that increases of pressure are linked to the increase of total mass within the model boundaries. If it were possible, the model domain would thereby be induced to expand. At the micro-scale, the bulk expansion arises from the fact that the rod components are squeezed by the added pressure acting on their exposed surfaces, and because of the geometry
of the rods, they attempt to elongate. However, as is common in the subsurface, if there are constraints that prevent the macro-scale expansion in some (or all) directions, then the stress components in all directions are increased when pressure increases (unless there is concurrent elongational bulk strain in one or two directions; that case is not addressed here, but was addressed in Couples 2019 and subsequent conference papers already mentioned). The fact that the fracture-normal stress increases, with no change in the related bulk strain, is already familiar within the subject of thermo-elasticity – where increases of thermal energy (increasing temperature) lead to ‘thermal stresses’. The point here is that a comparable response occurs due to the interaction between two distinct component types that comprise the solid skeleton, provoked by hydraulic loading acting on one component type (the rods).

The increase of stress that occurs due to a pressure increase is not (normally) observed in rock mechanics laboratory experiments, since a common protocol envisions the need to maintain stresses (e.g. radial confining pressure) at a constant value to facilitate the derivation of constitutive laws. The micro-scale model indeed calculates that there is a bulk expansion when pressure increases while the stresses are fixed – much like the expansion of a body with a temperature increase – if there are no constraints. In an experiment with a cylindrical sample, the expansion is expressed as an increase of the radius (and expansion in the axial direction if the experiment creates an isotropic stress state). In such an experiment, the radial displacements occur with no change of intensive energy within the skeleton of the sample, since the stress state is maintained at a constant value. In contrast, the micro-scale analysis shows that stresses cannot be constant in realistic subsurface situations where pressure changes occur in conjunction with dimensional constraints.

The processes envisaged in the sequence (below) are all, in principle, reversible. Thus, a real subsurface situation could evolve such that the state changes retrogress through a part of the list in reverse order, and there is equally the possibility to alter the evolution to a ‘forward’ direction, with the situation then progressing to higher-numbered steps. In a real-world setting, such variations in the loading sequence could conceivably occur in different places and at different times within some rock-mass region. The strict assumption of reversibility keeps the paper focused, but that choice eliminates a detailed consideration here of any processes that involve non-reversible steps (such as shear movement on the fracture, or texture changes induced into the matrix adjacent to the fracture, etc.). Such non-reversible changes are not well suited to the existing analytical micro-physics formulation, but they could be addressed via comparable numerical methods, and that is the subject of a future paper.

A series of ‘loading steps’, summarised as a numbered list, provides a framework for deriving the micro-scale states necessary to describe the evolution of fracture aperture:

1. The starting configuration involves the presence of a pre-existing fracture in a closed state. The subsequent loading steps examine the processes required to transition towards a critical state from which the fracture aperture evolves on a different pathway from previously. The prior strain state of the material point in the closed-fracture condition is the reference against which the subsequent strain states are referenced.

2. Fluid pressure is increased (this step is included to illustrate the roles of pressure change only, which could equally involve a pressure decrease). The closed fracture aperture does not change in this step.

3. Bulk strain, normal to the fracture, lowers the fracture-normal stress to zero. At that critical point, the aperture evolution changes trajectory.

4. Fracture opening. This transitory loading step involves interactions that exchange energy between fluid and solid. The energy transfer implies the action of additional far-field processes that are not captured by a description of the state variables alone.

5. For an open fracture, pressure continues to increase, causing the fracture aperture to increase because the matrix block shrinks in size.

6. Pressure diminishes (depletion of the fluids). In the ideal model arrangement, this step reverses relevant steps from the sequence already examined. This sequence could (but does not necessarily) reverse the model to its original state.
3.1 Loading step 1

As explained above, a closed fracture cannot become an open fracture until there is a reduction of the stress acting normal to the fracture plane, reducing it to a no-stress condition. The transformation of a closed fracture to an open fracture must involve a process explanation for the lowering of the normal stress. An obvious candidate for the reduction may be fracture-normal bulk elongation – in the configuration adopted here, that is expressed as $\Delta \epsilon_x < 0$ (such as the top image in Fig. 2). That strain also reduces the fracture-parallel stresses by a limited amount, because of the Poisson effect. Fracture-normal stress could also be reduced because of bulk elongation in one or both fracture-parallel direction(s), but the fracture-normal effects of that expansion are a small fraction of the reduction of fracture-parallel stresses, and also related to the Poisson effect. Unless the fracture-parallel stresses are already small in magnitude, in comparison with the fracture-normal stress, this potential effect is likely to have only a limited role, and it is not examined further here. Instead, it is suitable to focus on a single strain change (fracture-normal elongation) that can reduce the fracture-normal stress magnitude. Similarly, a reduction of fluid pressure is equally a possible process to lower the fracture-normal stress. Thermal changes (cooling) could also be involved, but those are not addressed in this paper.

It is worth noting that the size of the region, where elongational strain occurs, is not pre-determined. It has to be large enough that the micro-scale model is applicable, but that dimension is – perhaps – as small as the length needed to contain a small number of unit cells. That could be on the order of a centimetre (or less), and thus the strains could be very local and still have the effect specified. Of course, if the region with the altered state is small, then this fact implies strong local gradients, and the portion of the fracture with lowered normal stress might consequentially be small. Alternatively, the needed strain could be regional in scope, and affect rocks over distances of tens or hundreds of kilometres. The challenge of linking micro-scale physics to the real world is certainly not trivial. Later in the paper, a sensible context, for the necessary strains, is described.

3.2 Loading step 2

The expression (Eq. 1) that governs $\Delta F_x$ shows that the necessary bulk elongation is dependent upon both stress change and pressure change (and material parameters), although the effects of these are in opposition for positive changes in both. The amount of elongation strain needed to allow fracture opening (with no pressure change) is determined by rearrangement to calculate the strain that reduces the normal stress to zero (e.g. set $\Delta \sigma_x = -\sigma_x$). If pressure also changes, a minimum number for the required strain is obtained by setting $\Delta P = -P$. A larger elongational elastic strain is needed if $\Delta P > 0$; this could be addressed in combination with far-field elongation, or as a separate process that occurs before or after. As a reminder of the point made earlier in the paper, the necessary reduction of fracture-normal stress can also partly depend upon reductions of fracture-parallel strains, or by temperature reductions – but these options are not examined here, merely to retain the primary focus.

3.3 Loading steps 3 and 4

Although the transition examined in this ‘step’ is a crucial one, it does not depend on far-field changes. Instead, the transition from closed to open involves state changes in the micro-scale model that arise from a significant energy exchange that occurs between the pore fluid and the solid skeleton, with no alteration of the external states. Thus, there is an interesting phenomenon that must be understood, which takes place at the precise point in the process evolution where the normal stress becomes zero. The stress change of the skeleton is, in this instance, directly caused by the new loading of the truncated rod ends. This loading arises by means of the fluid pressure, when the fluid is able to wet these surfaces as they separate. Equation (1) defines the response of the matrix block. Here, the x-direction stress changes from $\sigma_x = 0$ to $\sigma_x = P$ at the ‘instant’ when the fluid loads the truncated ends of the rods. Thus, in Eq. (1), the terms are replaced accordingly as $\Delta \sigma_x = P$ and $\Delta P = 0$:
\[
\Delta \varepsilon_x = \frac{1}{E} \left[ P \left( \frac{1 - \nu + tv - 2\nu^2 + 4\nu v^2 + 2\nu^2 v^2}{(1 - \nu + tv)} \right) - 0 \left( \frac{2tv + 2\nu^2 - 2\nu^2 v^2}{(1 - \nu + tv)} \right) \right] \tag{3}
\]

Thus, for this increment of loading, the x-direction bulk strain is positive \( \Delta \varepsilon_x > 0 \) and so the block becomes smaller, and the fracture aperture increases because the matrix-block wall moves away from the similar block wall on the other side of the fracture plane.

Suppose, for convenience, that the fracture undergoes the virtual opening of its aperture ‘instantaneously’ (but ignore the momentum and inertia implications). Pore fluid fills the new void space between the truncated ends of the rods, or else the fluid could not exert the loading assumed. Where does that fluid come from? Can it invade that space in an ‘instant’? One idea is that the fluid comes from the adjacent matrix pore system, where the matrix pore pressure would have to diminish, at least for a time, so define this local, flow-related pressure change in the matrix as \( \Delta P = \Delta P_{flow} \) which is time-dependent. In the local setting, the pressure inside the fracture voids is smaller than the pressure in the matrix \( P_{fracture} < P_{matrix} \), and this is the gradient that provokes fluid motion.

Via Eq. (1), the increment of bulk strain caused by the reduction of pore pressure is negative,

\[
\Delta \varepsilon_x = \frac{1}{E} \left[ \Delta P_{flow} \left( \frac{1 - \nu + tv - 2\nu^2 + 4\nu v^2 + 2\nu^2 v^2}{(1 - \nu + tv)} \right) - \Delta P_{flow} \left( \frac{2tv + 2\nu^2 - 2\nu^2 v^2}{(1 - \nu + tv)} \right) \right] \tag{4}
\]

hence the matrix block elongates in the x-direction. Here, the case is illustrated where the change in the fracture pressure is the same as the change in the matrix pressure, as a limiting case that allows the following argument. The reasoning here is that the ratio of stress change to pressure change, for the condition of no strain change, is approximately 0.1 to 0.2 (Fig. 3). Since the ratio of actual stress change to pore pressure change, in this loading increment (Eq. (4)), is exactly (or nearly) 1.0, where the reduction of both terms is due to Darcy flow in the matrix to the fracture voids, the ‘stress term’ effect in Eq. (4) dominates over the ‘pressure term’. So, the region of matrix adjacent to the fracture plane expands and tends to close the fracture due to the flow. This response counters the opening caused by the pressure acting on the now-exposed truncated rod ends.

Where is the resulting position of the matrix wall? If it is assumed that the transient pressure reduction has been overcome, by means of fluid inflow occurring over some time period, and arriving to the region around the fracture from locations further into the matrix, then the strain calculation of Eq. (3) describes the matrix strain at the end of the transient. The aperture change is then a function of the length over which the strain is applicable. If the strain varies along the fracture-normal direction, then the displacement of the fracture wall is determined by integrating the variable strain over the length. In the example depicted in Fig. 1, with a set of parallel fractures that define individual matrix blocks of a consistent size, the aperture change is equal to the strain increment times the block dimension. This statement assumes that half of the length-change of each block is assigned to each of the two bounding fractures, and each fracture aperture is composed of two such contributions. If, as in the examples of fractured rock-masses introduced in the Discussion, the strain distributions are complex, then the estimation of aperture change is likely to require more sophistication, and may well necessitate a suitable numerical solution.

3.4 Loading step 4

Once the fracture opens, the fluid pressure in the void space of the fracture \( P_{fracture} \) loads the exposed ends of the half-length rods that form the face of the matrix block. The local conditions of \( \sigma_x = P \), and \( \Delta \sigma_x = \Delta P \), apply in all subsequent processes that occur while the fracture remains open:

\[
\Delta \varepsilon_x = \Delta P \frac{1}{E} \left[ \frac{1 - \nu + tv - 2\nu^2 + 4\nu v^2 + 2\nu^2 v^2}{(1 - \nu + tv)} \right] \tag{5}
\]

The micro-scale model provides a means to calculate the magnitude of the fracture-normal stress, which – at least locally, close to the fracture – cannot be independently inferred from macro-scale assumptions. And further increases in pressure cause the adjacent matrix to shorten, resulting in a further increase of aperture. Equally, the increase of \( \sigma_x \) causes an increase in the fracture-parallel stresses within the
matrix, if the no-strain conditions continue to apply in these directions. In situations with an already-open fracture, the state described here could be the appropriate starting point for many engineering analyses.

3.5 Loading step 5

Of course, Eq. (5) applies equally to the reverse case, where pressure is reduced while a fracture is already open. Such a pressure reduction could occur due to human-related removal of fluid energy, or it could be entirely natural – the micro-scale model is equally applicable. Whether a fracture may exactly reverse its opening history is dependent on the occurrence of behaviours that are dissipative, such as shear movement along fractures, or other possible changes. Those non-reversible events must be considered before making the assumption that the inherent reversibility of the micro-physics is an appropriate response to adopt. Another important consideration is the case where bulk strain has occurred, from non-local causes. If this change is part of the evolution, then the cumulative strain must be updated by means of Eq. (1), which also allows for changes in fluid pressure that may have occurred during the bulk strain process. Then, the question of strain during pressure reduction alone can be calculated via Eq. (5).

4 Discussion

The Discussion Section is divided into five sub-sections. The first assesses the similarities and differences between the micro-scale model and the commonly-adopted continuum-based models. The next sub-section examines the idea of effective stress, with a focus on the unhelpful perspective on stress states that is the consequence of reliance on process explanations based on effective stress. The third sub-section is a brief outline of the complex stress states that emerge in discontinuum geomechanics models of multi-fractured rock-mass systems, and emphasises how such systems provide the macro-scale circumstances for fracture aperture opening and evolution, as identified by the micro-scale method. The fourth sub-section considers the extension of the micro-scale understanding to the case of fractures that are ‘imperfect’, and whose characteristics are not as simple as the idealised arrangement adopted in the micro-physics formulation. A final sub-section looks at the perspectives for further application of the micro-physics approach.

4.1 Assessing the model

The general micro-scale model (Couples 2019) is constructed from three expressions that define the bulk strain in each of the three principal directions. The bulk strain is a weighted average (using the parameter $t$ that defines the relative length of rods to junctions) of the separate strain states that exist in the two types of skeleton components: the rods and junctions. Pore pressure loads the lateral faces of the rod elements, and thus defines the resulting lateral normal stresses in the rods. Assumptions about principal stresses, or strain constraints in up to three principal directions, allow the general model to be manipulated to derive an expression like that given as Eq. (1). For the application of this paper, that expression – which gives the relationship between the x-direction bulk strain, the x-direction principal stress, and the pressure, e.g. $\epsilon_x = f(\sigma_x, P)$ – is the complete ‘model’, although additional expressions can be derived to give the principal stresses in the other two directions (not needed here).

The model itself does not have a plane of discontinuity. The idea of a fracture plane that passes through rod elements, and indeed, the depiction of the lattice for the matrix material, are merely visual aids to assist in manipulating the model expression so as to be able to calculate the correct response of the porous rock that is here called the matrix. The introduction of the plane of discontinuity allows the model’s behaviour to be translated into movement of that bounding plane, by means of the strain and a separate input of the block dimension (from the reference point in the centre of the fracture from which the wall displacement is figured). It also provides a visual image of where and why the changing boundary conditions come into being. Regardless of these caveats, the visual images are relevant to assist in translating the model’s responses into information that is meaningful at the macro-scale.

An important point about the micro-scale model is that it calculates macro-scale responses that are comparable to those of classic continuum-based theories, and recovers parameters like Biot’s coefficient $\alpha$ (Müller et al. 2022), in loading cases which have stress
boundary conditions. But, the micro-scale model departs from continuum-based models in all situations which involve displacement (strain) constraints. This difference arises because continuum-based models of poroelasticity are developed as an extension of solid elasticity, wherein the additional ‘extended’ parameters come from laboratory experiments that are operated with stress boundary conditions. In any poroelasticity theory that includes parameters for the alterations of stress, as a function of pressure, those parameters are derived by arguments which assume that the solid behaves like an elastic solid – which is different to what the micro-scale model reveals. There is no simple way to make direct comparisons between the full range of behaviour of the micro-scale model, and the types of expressions that constitute the class of poroelastic models.

At present, there are no experimental tests of the micro-scale model, because it has proven impossible to design a laboratory configuration that can detect and measure skeleton stresses that are induced by fluid pressure, when the skeleton is prevented from experiencing strain. Thus, the micro-scale model is asserted to be compatible with fundamental physics in a simple, discrete model system, and thus it is inferred to be valid until demonstrated otherwise, or when confirmed if appropriate experimental methods are developed.

One important limitation of the micro-scale model is that it is formulated in principal coordinates, partly motivated by the adoption of the rectilinear lattice visualisation. In the lattice, there is a clear meaning of the parameter \( t \), which serves as a weighting factor for the contributions of the different element types of the skeleton. In a numerical simulation involving a realistic skeleton (such as seen in Fig. 1), it should be possible to load the model with shear on the boundaries, so the outcomes can be used to develop a complete material response. In such a numerical simulation, the identification of element types is less obvious, and it may well prove that a parameter similar to \( t \) appears as a ‘fitting’ factor that serves to provide a link to the observable texture of the solid elements.

4.2 Is effective stress an effective concept?

In poromechanics, the idea of effective stress has long played a key role (Lade and de Boer 1997). This idea is often described as arising first with the soil-mechanics (oedometer, thus uni-axial vertical loading) experiments of Terzaghi (1923), who posed that a laboratory parameter, comprising the numerical difference between the vertical stress and the pore pressure, e.g. \( \sigma = \sigma_v - P \), provided a convenient means to rationalise a suite of experimental observations (soil mechanics oedometer tests). Nearly a decade earlier, Fillunger (1913; 1914; 1915) had made similar experimental observations, but had not spelled out in quite the same clear manner his idea, as did Terzaghi later. More than a decade after Terzaghi’s initial publication, both of these engineers elevated the idea of effective stress into the basis of a 3D constitutive law (Fillunger 1936; Terzaghi 1936). In rock mechanics research (and operational practice), the concept of effective stress played a major role in the seminal engineering paper on hydraulic fracturing by Hubbert and Willis (1957), and in a similarly-influential paper on the mechanics of thrust faulting (Hubbert and Rubey 1959). Hubbert’s understanding derived from extensive experimental studies that were underway in the Shell Bellaire Research Lab (for which Hubbert had been the main instigator), and this foundation work was later published by Handin et al (1963). One of the key underpinning papers of modern poroelasticity, by Biot and Willis (1957), is still another example of the significant conceptual advances in poromechanics that emerged from the team associated with the Shell Lab in that timeframe. Subsequently, the concept of effective stress has become pervasive throughout rock mechanics.

The concept of effective stress is widely adopted in the analysis of slip on discontinuities, and especially in relation to ‘instabilities’ associated with fluid pressure perturbations, as witnessed by the treatments in numerous textbooks (Hobbs et al. 1976; Ramsay et al. 1987; Mandl 1988; Price and Cosgrove 1990; Jaeger et al 1999; Zoback 2010; Fossen 2016). The majority of such textbook explanations present this idea by means of Mohr-circle diagrams, within which increased pressure translates the Mohr-circle of stress towards the origin, until the circle contacts the failure surface. These process explanations do not usually account for the sometimes subtle interplay between sliding on old frictional surfaces in competition with the creation of new failures (Handin 1969). But, more importantly, the textbook explanations rarely acknowledge any alteration of the state of stress associated with pressure change. There is another suite of
views that see fracture apertures as being governed by the state of effective stress (Walsh 1981; Gale 1982; Bai et al. 1993; Ghabezloo et al. 2009), which equally seem to assume that the state of stress is independently fixed without a dependency on the variable fluid pressure.

The micro-scale perspective elucidated in this paper strongly disputes the attitude that a subsurface stress state can remain constant during a change of pressure. This disparity warrants a consideration of the idea of effective stress, using the behaviour of the micro-scale model as the basis. It is noted in this paper that the normal stress must reduce to 'zero' on a closed fracture, for it to be able to open. By simple algebra, the effective normal stress thus becomes negative during the progress towards zero normal stress. Can the condition of negative effective stress exist in a rock material, without provoking that material to fail? Here is not the appropriate circumstance to undertake an exhaustive analysis. Instead, some elementary thought experiments serve to frame a later and extensive discussion that will be informed by the understanding arising from the micro-scale model.

Imagine a small block (say, 1 cm$^3$) of porous rock that is situated within a pressure vessel. The apparatus is dry at the beginning of the thought experiment. The sample is suspended in the vessel (which can be readily achieved in a thought experiment), and thus is not subjected to any mechanical parts that provide loads to its boundaries; therefore, the sample initially possesses no stress (ignoring the slight distortion of the sample due to gravity). The cube of rock comprising the sample subsequently is immersed in water, achieved by filling the vessel, and the pore system of the rock becomes fully saturated. Now, the water is pressurised. What is the resulting state of stress? What is the resulting state of effective stress?

From the classic continuum-based perspective, it could be suggested that the sample has a null state of stress since it is not loaded by any mechanical device. That view would lead to the interpretation that the effective (isotropic) stress is negative: $\sigma' = 0 - P = -P$. Alternatively, it could be posed that the sample’s state of stress is equal to the pressure of the surrounding fluid, inferring that the pressures on the sample face create the same stress internally. In this view, the effective stress is zero: $\sigma' = P - P = 0$.

What does the micro-scale approach reveal about the states of the sample?

Following from the assumption adopted earlier in the paper, the micro-scale stress in the axial direction of each rod, and in all three directions in the junctions, is assumed to be equal to the macro-scale stress, and in this case, the boundary conditions are given as:

$$\Delta \sigma_x = \Delta \sigma_y = \Delta \sigma_z = \Delta P$$

with transverse stresses in all of the rod elements also equal to the pressure:

$$\Delta \sigma_{\text{rod}}^{\text{transverse}} = \Delta P$$

Thus, in all parts of the skeleton, the principal stresses are equal to $P$, and the classic view of effective stress gives the answer that $\sigma' = 0$.

However, the loads from the pressure create a bulk strain (here expressed for the x-direction, with all directions being equal in this loading), which is composed of axial strains in the rod and junction elements (see the Appendix for the background to these expressions; this derivation is also in Couples (2019)):

$$\Delta \epsilon_{\text{axial}}^{\text{rod}} = \frac{1}{E} \left[ \Delta \sigma_{\text{axial}} - \nu(\Delta \sigma_{\text{axial}} + \Delta \sigma_{\text{axial}}) \right] = \frac{\Delta \sigma_{\text{axial}}}{E}(1 - 2\nu)$$

$$\Delta \epsilon_{\text{axial}} = t \Delta \epsilon_{\text{axial}}^{\text{rod}} + (1 - t) \Delta \epsilon_{\text{axial}}^{\text{junction}} = \frac{1}{E} \left[ \Delta \sigma_x(1 - 2\nu + 2\nu t) - 2\nu t \Delta P \right]$$

This expression is valid for any value of the isotropic stress state. In the case here, the boundary stress condition is $\Delta \sigma = \Delta P$, therefore, the bulk strain is given as:
\[ \Delta \varepsilon_x = \frac{1}{E} [\Delta P (1 - 2v + 2vt) - 2vt \Delta P] = \frac{\Delta P}{E} (1 - 2v) \quad (11) \]

which indicates a uniform shrinkage for a positive value of pressure, with \( \Delta P > 0 \), because the pressure changes from zero to \( P \). This calculated value defines the principal strains of an isotropic contraction, and is equivalent to what is anticipated from the continuum perspective. Therefore, if the problem constraints are specified as an isotropic stress state, the micro-scale model gives an answer that is the same as comes from the continuum view. In the uniaxial-strain conditions that are adopted for the fracture case, the equivalent expression for the un-controlled strain direction, with \( \Delta \sigma_x = \Delta P \), is:

\[ \Delta \varepsilon_x = \frac{\Delta P}{E} \left[ \left( 1 - v - tv - 2v^2 + 4tv^2 + 2r^2v^2 \right) \right] \quad (12) \]

For all valid parameter combinations (of \( v \) and \( t \)), Eq. (12) indicates a smaller contraction than does Eq. (11).

Although the idea of effective stress has no meaning at the micro-scale, where the solid and void spaces are separate elements of the model, the responses of the micro-scale model can be presented in terms of effective stress. The problematic aspect of effective stress is not the idea itself, but the ways that the concept has been applied – by assuming the constancy of stress state. That perspective is (probably) correct in many rock-mechanics experiments, but it is almost always incorrect in subsurface applications, where strain controls lead to the appearance of stress changes for almost every conceivable situation where there is a change of fluid pressure. The circumstances where constancy of stress might apply include the case of a matrix block, separated from other blocks by open fractures (in some directions). Based on the arguments made herein, the fracture-normal stresses might be approximated by the fluid pressure in that setting – but that inference ignores the roles of non-constant-value displacement discontinuities along other boundary surfaces, such as bedding planes, and how those effects are distributed through a block of fracture-bounded matrix. Such complexities are suitable topics for additional examination, but that effort needs numerical tools that encapsulate the ways that process interactions (solids and fluids) become expressed at the macro-scale.

4.3 Discontinuum geomechanics of fracture arrays

The macro-scale implications of the micro-scale model, especially the need for reduction of the normal stress to zero magnitude for a fracture to open, might seem unusual in relation to common views that see stress states as being regionally consistent and totally compressive (Hickman 1991; Zoback 1992; Engelder 2014). Equally, there are those views which assign fracture-aperture dependency on the state of effective stress, which equally treat the stress as a constant (Walsh 1981; Gale 1982; Bai et al 1993; Ghabezloo et al 2009). Is there a macro-scale perspective on stress-state changes that reshapes the form of these topics?

Understanding that has been developed for fractured rock-mass behaviours, using a discontinuum geomechanics approach, reveals spatially-complex stress states when systems of fractured rock are subjected to far-field loadings. Such simulations are formulated by envisioning the rock-mass as being composed of discrete blocks that contact and interact with adjacent blocks. Within an individual block, the rules of continuum are assumed to apply, and the interfaces or places where adjacent blocks touch obey contact laws that can be described as ‘frictional’ in nature. This paper is not the appropriate place to undertake a full critique of their numerical formulations nor the fundamental expressions involved, especially since none of the existing methods acknowledge the implications of the micro-scale process interactions that are the focus of this paper. Instead, the examples are presented to illustrate the extreme heterogeneity of states that evolve as the simulated systems develop in their highly non-linear ways. The simulation outcomes provide an insight into a subsurface context that may be important for making full use of the micro-scale understanding described in this paper.

The geomechanical perspective adopted in these examples is that of a pre-fractured rock-mass which is subjected to some new arrangement of boundary loads. The simulated responses consistently indicate that such a rock-mass model develops spatially-complex, and varying, geomechanical states. The non-uniform states reveal some places with local complete unloading (even macro-scale openings, if the formulation enables that), along with local reductions of stresses, and with local stress increases in some parts of the model domain. These are exactly the types of
local states that are identified in this paper as being necessary to cause opening and subsequent changes of fracture apertures in response to both geomechanical and fluid perturbations.

Baghbanan and Jing (2008) employ UDEC™, and reveal the upscaled responses of systems composed of many blocks bounded by frictional discontinuities. An example from their study (Fig. 6A) shows the spatial complexity of the states of stress within the rock-mass, revealing regions that are nearly unloaded, along with a distribution of principal-stress orientations that are not similar to the boundary conditions. A simulation by Hall et al (2007), using SAVFEM™ (see Couples et al 2007), where the full domain consists of a complete continuum partitioned by narrow zones of reduced-modulus continuum (these zones serve as proxies for large-scale fault zones), shows a similar arrangement of unloaded regions and highly non-uniform principal stress orientations and magnitudes (Fig. 6B). These models lead to an interpretation that the presence of narrow bands of easy-shear capability allow a rock-mass to respond in ways that are wholly unlike those expected of a comparably-sized block of continuum.

Discontinuum-based simulations reveal that – within a fractured rock-mass – it is to be expected that stress states (and the underlying elastic strains) are spatially variable, and may change as loading evolves. This is precisely the context that is identified as necessary for aperture opening, and aperture changes, via the micro-scale analysis. When combined with a trend of pressure increase (perhaps during reservoir filling), the circumstances within a fractured rock-mass may provoke quasi-local bulk volumetric changes that, in turn, represent the type of ‘loads’ that the discontinuum simulations employ to create the micro-scale local variations that lead to local aperture changes. The discontinuum simulations reveal that even within one fracture-bounded block, the stress states vary considerably. Thus, the ‘bulk strain’ changes identified by the micro-scale analysis, as being necessary in the matter of fracture opening, may occur on scales as small as within an individual block of matrix.

4.4 Considerations towards greater realism of fracture characteristics

The development of the analytical micro-scale model demands some geometric simplifications. Extending that model to address the role of a fracture, as reported in this paper, requires the acceptance of a further simplification in terms of the characteristics of the discontinuity that represents the fracture. Is it possible to employ the micro-scale-derived behaviours, and the resulting macro-scale responses, in such a way that they lead to understanding of more-realistic fractures? In this sub-section, two aspects of the real-world geometric ‘imperfections’ of fractures are briefly examined to assess what micro-scale
understanding can be applied. This analysis considers, in turn, fractures that have broken fragments within their void space, and macro-scale fractures that exhibit a transition from closed to open along the fracture surface.

The void space of real fractures may be partly filled by solid components, such as precipitated minerals, tarry components deposited from a hydrocarbon phase, or fragments of the wall rock (or of damaged mineral precipitates). It is clear that in such circumstances, the idealised picture – of an open void – is incorrect. The example illustrated is a real fracture that contains a distribution of fragments that are sourced from the adjacent matrix material, associated with slight shear motion along the fracture surface (Fig. 7). This example occurs within a rock sample deformed under experimental conditions, so the interpreted genesis of the observed textural elements is sufficiently constrained for the purpose here.

For the texture shown, it is simple to infer that – if this sample were located in the deeper subsurface – fluids would be expected to fill the pore spaces between the fragments, as well as the pores in the adjacent matrix rock. The fluid pressure would, in that situation, define a pore pressure as well as a fracture pressure. Indeed, this sample is employed in neutron tomography experiments that directly observe fluid flow processes (Tudisco et al. 2019; Lewis et al. 2022), which confirm that aqueous fluids both enter both the matrix regions and the fracture fill material, during water imbibition into the air-filled sample, as well as water flow through much of the pore system after the sample is fully saturated.

What does the infill imply in relation to the micro-scale analysis? Although the analytical model cannot directly accommodate this ‘anomalous’ micro-scale textural variation, the role of real-world infill is to allow the fluid pressure to act on the ends of the truncated rod-like elements. The infill serves also as a material with stiffness, and so the walls of the fracture cannot converge into a void space. Instead, the elastic energy of the porous infill is in equilibrium with the elastic energy in the adjacent matrix blocks. Thus, the matrix blocks are characterised by a compressive normal stress while the infill is compressed. The inference is made that, while the normal stress continues to exceed the magnitude of the pressure, the fracture does not open (no further than its partial prior opening necessary to contain the infill material). That inference is based on the potential energy analysis described in the earlier text associated with Eq. (1). However, when the bulk strain (normal to the fracture) reduces the normal stress so that it equals the pressure, the response is inferred to be a maintenance of the local state that permits this fracture to open its aperture exactly by the amount linked to the

Fig. 7 SEM image of an experimentally-created discontinuity in a fine-grained carbonate rock. The crystal size of this micrite sample is a few microns, now largely cemented into a solid skeleton. The deposition produced laminations of approximately 1 mm thickness (indistinct and oriented vertically in this view), with each of the two dominant types exhibiting contrasting pore-space characteristics. The induced deformation creates a dilated zone that is partly open space, and is otherwise partly filled with broken fragments of the original rock. The deformation feature serves as an example of complex local textures within a ‘fracture’, as well as non-planarity of the overall shape. Image courtesy of Dr Jim Buckman and Dr Helen Lewis. See Tudisco et al (2019) for a description of flow experiments that utilize this sample.
bulk strain changes and the block size (per the discussion under Loading Steps 3/4). The normal stress then equals the value of the pressure. This circumstance avoids the energy ‘crisis’ that is described in Loading Step 3. In a rock-mass with both ‘clean’ and filled fractures, there may be multiple factors that govern the resulting evolution of aperture changes.

The next real-world circumstance to examine is one where – along the mid-plane of a single fracture – a part of that fracture (Fig. 8) is closed (and clean), and an adjacent part is already open (for whatever reason, such as a difference in the normal strains already experienced). An alternative for the ‘open’ part of the fracture is that its prior history created an aperture that is now filled with an aggregate of solid particles whose interstices create a very local pore system (as described in the preceding paragraphs). Maintaining the quasi-static perspective, the pressure is equal in both matrix blocks adjacent to the fracture, in both positions along the fracture, and within the fracture itself (including within the porous infill of that version of the ‘open’ fracture). Based on the analysis earlier in the paper, the fracture-normal stress where the fracture is open is equal in magnitude to the pressure. Where the fracture is closed, the fracture-normal stress is some other value that might be near zero.

Consider a new loading increment where the bulk fracture-normal strains do not change ($\Delta \varepsilon_n = 0$), while the pressure is increased ($\Delta P > 0$). The micro-scale model (with the constraints adopted in this paper) can be employed to estimate the local responses in both locations (material points A and B) along the fracture, but this simple analysis does not account for any long-range interactions between the locations that might occur due to changes of state at these places. In the location where the fracture is open (material point B), the increase of pressure causes the local aperture to increase (slightly), and (slightly) increases the fracture-parallel stresses. At the closed location (material point A), the increase of pressure leads to an increase in the normal stress, along with increasing the fracture-parallel stresses, and the fracture remains closed.

What changes take place at points that are positioned between the two already-examined locations on the partly-open fracture? In the image (Fig. 8), the matrix rock on one side of the fracture plane is depicted in a 2D slice. The position of the fracture/matrix wall is shown as a dashed line, for its previous position, and by a solid line, for its new configuration after the pressure is increased. The position of the fracture/matrix wall is depicted as a smooth shape at this scale, with a slight curvature. This bounding surface needs to be tangent to the fracture medial surface in those places where the fracture is closed, and it is drawn parallel to the fracture medial surface at material point B.
Because of the change of shape (dashed line to solid line), the curved face of the matrix becomes more curved (across this field of view) when the aperture increases in the open portion of the fracture. The change of curvature is interpreted as a type of bending process, and thus, the outer arc of that bending (i.e. immediately adjacent to the face of the matrix) is slightly elongated (indicated by the exaggerated changes of ‘strain markers’ depicted on the drawing) at locations near material point A - and contraction near material point B. Such elongation//contraction represents a bulk strain that takes place approximately parallel to the fracture. If this occurred in a dry, solid, continuum case, it would be accompanied by a reduction or increase (respectively) in the state of stress parallel to the fracture. By the Poisson effect, the other stress parallel to the fracture would also be reduced/increased. In an isolated layer, the normal stress would also reduce/increase. The part of the fracture near the closed aperture would experience this reduction of normal stress, while the already-open part would continue to have a normal stress equal to the pressure.

In the micro-physics models, at the closed and open locations, the changes created by this ‘large-scale’ bending lead to a reduction of elastic potential energy within the elements of the relevant lattice model, even though the normal stress is held constant (equal to pressure) in the micro-physics model where the aperture is open. Perhaps the most interesting thought to be provoked is that the elastic potential energy at the closed location is affected by both the pressure change, and by the bending strains inferred to be linked to the increase of open aperture. It is possible to imagine that the bending effects could allow the open portion of the fracture to advance into what was previously a closed portion of the fracture. This would, in effect, amount to a propagation of the fracture opening.

As noted earlier in the paper, the question, of how much displacement occurs at the solid//fluid interface, is not solvable merely by asserting that the pressure and stress parameters have any particular numerical value. The effects of the bending deformation equally alter the model expressions, since the constraint conditions are now not fixed, but instead are dependent upon a particular context that is not well-described by an arbitrary bulk strain value. The several-context interactions described here mean that the problem demands a formulation that is based on a full energy budget (as discussed earlier). Even with the simplicity of the lattice model, the multiple effects imagined here lead to complicated expressions that involve recursive dependencies, and the resulting non-linear forms cannot be easily solved by simple algebra. A numerical analysis of the idea posed will be the subject of a future publication.

4.5 Perspectives

The analytical micro-scale model provides a means to calculate the consequences – at both the micro-scale, and in terms of bulk macro-scale responses – of fluid//solid-skeleton interactions. Very importantly, the model demands an approach which requires the user to examine the way that the problem is specified, and to recognise that there is little understanding gained by assigning fixed stress boundary conditions. Thus, to use the model may necessitate an alteration of the mind-set that might otherwise be adopted.

In this paper, the micro-scale model is employed so as to calculate a bulk strain normal to a putative fracture – and the result is used to make situational inferences. In this usage, where there is a ‘free’ face, that approach may be justified. However, in the preceding sub-section, a non-local interaction is described that introduces the possibility that other boundary conditions (fracture-parallel strains) can no longer be comfortably taken to be fixed. This example highlights that state parameters are not sufficient as the basis to solve complex problems. This is because state parameters are the dependent variables, and their values indicate the outcome of a process.

Extending this point: consider two differently-defined micro-physics models (contrasting values of $E$, $v$ and $t$) that are situated side-by-side. The problem is to define the movement of the common interface between the two models – in, for example, the problem constraint where their other boundaries are fixed. This problem is not solved by the specification of state parameters, as shown in this paper. Instead, it requires a full energy budget, which may well involve mass exchange at least for the fluid. This statement may be better stated as that there is energy exchange across the boundary of the model under examination, as well as movement of the interface. And this two-block problem can be expanded to imagine one micro-scale model surrounded by others, that are
surrounded by still others. In that arrangement, which is the fundamental description of a classic finite element model domain, all of the constraints are absent within the domain interior. In such a formulation, the displacements of the block (‘element’) interfaces are determined by the numerical solution.

Thus, the ultimate task is to develop a means to translate the range of micro-scale understanding (which may be considerably larger than described herein) into formulations that operate like classical continuum-based systems, where the solutions within the interior of the domain are derived via a complete energy formulation. As illustrated in this paper, the energy contents of micro-scale models differ from those of an equivalent continuum-like model in all circumstances where displacement constraints occur, and especially in all circumstances that involve pressure change. Since mutual displacement constraints occur everywhere in a discretised problem domain, there is a profound difference between the material concepts attached to the micro-scale perspective, and those asserted to represent an enriched-continuum material. The creation of such a micro-scale-based method, which is capable of solving large-scale system interactions, will permit the understanding developed in this paper to be re-assessed without the need to accept arbitrary assignments of constraints or states.

5 Conclusions

An analytical micro-scale model, based on a simplified digital-rock model that is a discrete depiction of the solid skeleton and the void space, provides a means to calculate the reversible, bulk response of a material point, based on a coupling between geomechanics and pore pressure. The resulting upscaled behaviour of such a model provides the basis for calculating appropriate laws for a material point composed of matrix rock. This paper extends the micro-scale concept examined previously, by the adding a free face, thus forming a micro-scale representation of the local matrix/fracture interface.

The analysis reveals the micro-scale interactions that govern how a closed fracture transitions to an open fracture (one with non-zero aperture). A closed fracture does not become an open fracture by pore pressure increases alone. Instead, bulk elongation normal to the fracture is necessary to reduce the fracture-normal stress to zero, so that the fluid may enter into the previously-closed fracture. The bulk strain can be created from tectonic causes, or by the multi-block responses characteristic of a rock-mass containing arrays of discontinuities, or potentially by other macro-scale processes not examined here. Once open, a fracture’s aperture can be increased by increasing the pore pressure, and its aperture will reduce with a pressure reduction, and possibly close.

In the example of a fracture that contains broken material, which constitutes a micro-porous medium (gouge) within the fracture void, the role of fluid pressure is slightly different. In this circumstance, once the normal stress is reduced to equal the pore pressure, the fracture thereafter opens according to the rules identified by the ideal fracture case. In the case of a fracture which is partly closed and partly open, macro-scale reasoning poses the idea that the flexing of the wall-rock further affects the local states via alteration of the fracture-parallel strains.

These extensions of the understanding, derived from uniform-state micro-physics, point to the need to develop new simulation methods that can accommodate the more-complex micro-scale states implied by the non-local situations that may arise in rock-mass evolution.

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Declarations

Conflict of interest The author has no competing interests to declare that are relevant to the content of this article.
Appendix

Background of the micro-physics model

The micro-physics model adopted here has its origins in the subject of digital rocks, wherein micro-scale 3D representations of the textures of porous geomaterials are employed to calculate or simulate fluid-flow processes (Bakke and Øren 1997; Blunt et al. 2012; Andrä et al. 2013; Bultreys et al. 2016; Jiang et al. 2018; Zhao et al. 2019). In the majority of these methods, the skeleton of the model is treated as fixed framework that merely ‘hosts’ the pore space – the exceptions involve approaches that investigate the wettability of the solid surface, but these still employ the fixed geometry. Whole-model (bulk) outcomes from such fluid-flow simulations provide the basis to derive continuum-scale values for the ‘properties’ that are necessary for understanding and quantifying multi-phase fluid-flow processes (intrinsic permeability, relative-permeabilities, and capillary pressure curves). These macro-scale characteristics are obtained via upscaling the process outcomes of the micro-scale simulations.

This paper employs a comparable approach, but with the focus here being on the quasi-static interactions that alter both the solid framework and the pore system, and which reveal the coupling of the roles of geomechanics and fluid pressure. This approach involves an important modification of the previous digital-rock model paradigm: the skeleton is no longer treated as fixed, but, instead, it deforms via reversible (elastic) responses. The analytical functions developed in this approach define changes of physical-states that represent the bulk (or upscaled) poromechanical response of the digital rock model (Couplès 2019). The formulation thus determines the responses of a ‘material point’ via a discrete aggregation of the micro-physics behaviours that are the responses to imposed alterations of the physical states.

The solid skeleton of the rock, and its space-complement, the pore system, are distinctly represented in the model, but the version adopted here simplifies the real geometries of a rock skeleton and its pore system into reticulated networks that together fill the space of the model domain. This simplification allows the multiple physical states within the skeleton to be calculated via analytical expressions; this enhances the transparency of the method, while revealing the essential process interactions that persevere in spite of the reduced geometric complexity inherent in this approach. The consequential simplification of the pore-system geometry is not suited to the purpose of simulating fluid flow processes, but in the quasi-static perspective adopted here, that is not an important limitation.

A realistic skeleton is always a multi-connected network composed of solid elements, with a topology and geometry that is the space-complement of the similarly-complicated pore network. In the early stages of pore-network modelling for fluid-flow simulations, real pore networks were simplified into regular, reticulated arrays with uniform-length connections between junctions (McDougall et al 2002). The sizes of connecting elements and of the junctions could be assigned arbitrarily, and these flow-significant parameters provided the means by which such a model could be adjusted to represent different porous materials.

In spite of those simplifications, the resulting flow simulations were able to incorporate pore-scale physics that was derived from true-scale 2.5D physical models of pore systems (this is now widely called ‘micro-fluidics’ in many industrial settings), which involved video recording of the real multi-phase fluid movements under realistic pressure and temperature conditions (Sohrabi Sedeh et al 2000). In spite of the geometric simplifications, the early pore-network models were able to be ‘tuned’ to limited descriptive data, and then used to make flow predictions for other governing conditions that could be verified by means of the experiments. Thus, the
geometric simplifications did not destroy the fundamental behaviours of multi-phase fluid interactions and movements.

Subsequently, modern pore-network flow simulations utilise the real observed geometries of pore systems (Ryazanov et al. 2009), while continuing to evolve the sophistication of the underlying physics arising from theoretical and experimental work (van Dijke et al. 2004; 2007). Pore-network methods now permit the ab initio simulation of multi-phase fluid flows in very complicated pore systems that exhibit multi-scale pore elements (Jiang et al. 2013), materials with space-delimited variations of contrasting pore-system types (Jiang et al. 2018), and pore systems comprised of matrix rock materials of arbitrary complexity plus the addition of deformation features (Jiang et al. 2017). Such pore-network models of fluid flow play an important role in explaining and understanding the direct observations of fluid flow obtained via neutron tomography (Tudisco et al. 2019; Lewis et al., 2022).

Here, the adopted micro-scale model reverts to the simplified geometric arrangements that proved so useful in advancing the efforts on fluid-flow simulations (noted in the preceding paragraphs). The expectation is that the geometric simplifications, being employed now, will be replaced, in due course, by a transition to models with a high degree of geometric fidelity. The current reduced-complexity model arrangement portrays the solid skeleton in a geometrically-simplified way, where the solid configuration is in the form of a regular, reticulated lattice (Fig. 9). By means of this simplification, the equations of elasticity are readily expressed in each component part of the skeleton. These expressions include the role of fluid pressure, which acts on the surfaces of the skeleton that are in contact with the fluid-filled pore system.

The analytical model’s functional relationships (summarised below) are written with $\Delta$ symbols for each state parameter, to emphasise their intended use for examining the effects of changes in loadings. Fluid pressure directly loads the exposed faces of the skeleton and void system from a digital-rock model, such as the one depicted in B. D A unit cell of the lattice, with short rod elements typical of low-porosity materials. E Exploded view of the unit cell, showing the hidden junction (blue), the x-direction rods (orange), the y-direction rods (yellow), and the z-directions rods (green).
connecting solid elements (called ‘rods’), where the change of the relevant normal-stress component in a rod is set equal to the pressure change. However, the role of fluid-pressure change is felt throughout the lattice, since changes of state in the rods create changes of state in the ‘junctions’ which join the ends of the rods. It is worth emphasising that the junctions and rods do not have the same states of stress, due to the explicit treatment of the fluid pressure acting on the faces of the rods. These contrasting stress states are apparent (see below) in the formulation of the analytical expressions.

The analytical model has been described previously (Couples 2017; 2019), so the treatment here is deliberately brief. Examples of the use of the analytical model expressions, to derive the directional responses (changes in bulk strains or principal stresses) that are not specified by a given set of problem assumptions, can be found in Couples (2020; 2021a; 2021b; 2021c). The model is formulated via asserting that there is a single state of stress in each junction, and three states of stress in the three directionally-different rod elements. The pore elements are all at a uniform pressure, and the pressure acts directly on the exposed faces of the rod elements. The stress component normal to those rod faces is assumed to be equal to the fluid pressure acting on each face.

Linear, isotropic elasticity is assumed to characterise the mechanical response of the solid components (both rods and junctions). The coordinate directions of the lattice are assumed to be principal directions, so no shear terms appear in this simplified formulation. The constitutive equations of elasticity are arranged so as to agree with whatever far-field (boundary) changes of conditions are specified for a given problem (these consist of suitable sets for: directional stresses, e.g. \( \Delta \sigma_y \), bulk strains in each direction, e.g. \( \Delta e_x \), and the fluid pressure \( \Delta P \)). By algebraic re-arrangement, it is possible to derive expressions for an unknown state parameter, given as a function of the input state parameters, the material constants \((E, v)\); the Young’s modulus and Poisson ratio, respectively) of the solid skeleton material, and a ‘textural’ parameter \((t)\) that specifies the relative lengths of rods in a unit cell. Figure 10 shows the way that the parameter \(t\) relates to the porosity. These parameters appear in the expressions below.

For the problem posed in this paper, namely the question of the aperture change of a fracture located in the y–z plane, it is appropriate to derive an expression of the change of x-direction bulk strain as a function of the change of x-direction stress and the change of pressure (Eq. 13). The detailed algebra and associated justifications are presented elsewhere (Couples 2021a; 2021c), and only a summary is given here. The gist of the derivation is illustrated via the following key steps in the sequence:

\[
\Delta e_y^{\text{function}} = \frac{1}{E} [\Delta \sigma_y - v(\Delta \sigma_x + \Delta \sigma_z)] = \frac{1}{E} [\Delta \sigma_y - v(\Delta \sigma_z + \Delta \sigma_y)]
\]

\[
= \frac{1}{E} [\Delta \sigma_y (1 - v) - v \Delta \sigma_x]
\]  

\[
\Delta e_{y}^{\text{rod}} = \frac{1}{E} [\Delta \sigma_y - v(\Delta \sigma_x + \Delta \sigma_z)] = \frac{1}{E} [\Delta \sigma_y - v(\Delta P + \Delta P)] = \frac{1}{E} [\Delta \sigma_y - 2v \Delta P]
\]

Then, weighting the contributions of the rods and junction by the relative lengths, using the textural parameter \(t\):

\[
\Delta e_y^{t} \equiv 0 = \frac{1}{E} [(1 - t)(\Delta \sigma_y (1 - v) - v \Delta \sigma_x) + t(\Delta \sigma_y - 2v \Delta P)]
\]

Fig. 10 Relationship between the textural parameter \(t\) and porosity

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\[ \Delta \sigma_y = \Delta \sigma_z = \frac{\Delta \sigma_x(v - tv) + 2tv\Delta P}{(1 - v + tv)} \]  

(17)

Now, turning to the \( x \)-direction:

\[ \Delta \varepsilon_{\text{junction}}^x = \frac{1}{E} \left[ \Delta \varepsilon_x - v \left( \Delta \sigma_y + \Delta \sigma_z \right) \right] \]
\[ = \frac{1}{E} \left( \Delta \varepsilon_x - 2v \Delta \sigma_x(v - tv) + 2tv\Delta P \right) \]
\[ = \frac{1}{E} \left( \Delta \varepsilon_x - 2v \Delta \sigma_x \right) \]

(18)

\[ \Delta \varepsilon_{\text{red}}^x = \frac{1}{E} \left[ \Delta \varepsilon_x - v \left( \Delta \sigma_y + \Delta \sigma_z \right) \right] \]
\[ = \frac{1}{E} \left( \Delta \varepsilon_x - 2v \Delta \sigma_x \right) \]

(19)

\[ \Delta \varepsilon_{\text{aux}}^x = \frac{1}{E} \left[ \Delta \varepsilon_x \left( \frac{1 - v + tv - 2v^2 + 4tv^2 + 2t^2v^2}{1 - v + tv} \right) \right] - \Delta \sigma_x \left( \frac{2tv + 2tv^2 - 2t^2v^2}{1 - v + tv} \right) \]

(20)

\[ \Delta \varepsilon_{\text{aux}}^x = \frac{1}{E} \left[ \Delta \varepsilon_x \left( \frac{1 - v + tv}{1 - v + tv} \right) \right] - \Delta \sigma_x \left( \frac{2tv + 2tv^2 - 2t^2v^2}{1 - v + tv} \right) \]

(21)

The bulk strains of the micro-scale model provide an unambiguous link to the continuum-equivalent strains of the macro-scale material point associated with the micro-scale model. To define the cross-scale stress relationship – between the (directional//principal) stresses in the micro-physics model, and the (principal) stresses applicable at the macro-scale – requires both a clear definition, as well as a justification. Precisely: the coordinate-direction normal stresses that exist at the micro-scale, which are constant along each direction and continuous from a rod to the adjacent junction, are defined as being the identical with the apparent external stresses (or boundary states). This decision aligns with the status quo in experimental studies of rock mechanics, in which the stress state within a sample is taken to be the same as the apparent external state that is created by the actions of the confining medium and the axial platens (expressed for a cylindrical sample). Although there are reasons to question this particular sentiment (Couples 2019; 2021b), its adoption here provides a continuity with historical thought, and, moreover, the conclusions reached herein are not affected by making this choice. Thus, the micro-scale stresses that align with the lattice, and the macro-scale normal stresses, are considered to be equal.

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