Validation and Application of Iterative Coupling to Poroelastic Problems in Bone Fluid Flow

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Abstract—An iterative method for coupling fluid flow and mechanical deformation in porous media is presented. The iteratively coupled scheme of the STARS reservoir simulator was applied to three example problems: the Mandel-Cryer phenomenon; a bone specimen under cyclic loading; and a dual-material (continuum) example. Through these examples, the accuracy of the numerical scheme was confirmed, and the applicability of STARS as a sophisticated tool for the study of problems in bone fluid flow was demonstrated.

Index Terms—Poroelasticity, fluid mechanics, iterative coupling, bone.

NOMENCLATURE

\begin{align*}
  B & \quad \text{Skempton pore pressure coefficient} \\
  E & \quad \text{Young’s modulus} \\
  G & \quad \text{shear modulus} \\
  K & \quad \text{bulk modulus} \\
  M & \quad \text{bending moment} \\
  N & \quad \text{applied load} \\
  P & \quad \text{nondimensional pressure} \\
  T & \quad \text{nondimensional frequency} \\
  V & \quad \text{volume} \\
  Z & \quad \text{nondimensional thickness} \\
  a & \quad \text{length} \\
  b & \quad \text{height} \\
  c & \quad \text{diffusion coefficient} \\
  k & \quad \text{permeability} \\
  m & \quad \text{nondimensional bending moment} \\
  p & \quad \text{pore fluid pressure} \\
  q & \quad \text{Darcy fluid velocity} \\
  t & \quad \text{time} \\
  u & \quad \text{solid displacement} \\
  w & \quad \text{width} \\
  \alpha & \quad \text{Biot’s effective stress coefficient}
\end{align*}

\begin{align*}
  \varepsilon & \quad \text{strain} \\
  \mu & \quad \text{dynamic fluid viscosity} \\
  \nu & \quad \text{Poisson’s ratio} \\
  \rho & \quad \text{density} \\
  \sigma & \quad \text{stress} \\
  \tau & \quad \text{nondimensional time} \\
  \phi & \quad \text{porosity (pore volume fraction)} \\
  \omega & \quad \text{angular frequency}
\end{align*}

\begin{align*}
  i, j, k & \quad \text{components of the tensors in field equations} \\
  b & \quad \text{bulk} \\
  d & \quad \text{drained} \\
  f & \quad \text{fluid constituent} \\
  m & \quad \text{mean} \\
  p & \quad \text{pore} \\
  s & \quad \text{solid constituent} \\
  u & \quad \text{undrained} \\
  v & \quad \text{volumetric}
\end{align*}

\begin{align*}
  ^o & \quad \text{reference value} \\
  n & \quad \text{time level}
\end{align*}

I. INTRODUCTION

Bone is a complex, hierarchically organized biomaterial that serves important biomechanical and metabolic functions. Bones have remarkable structural efficiency and continuously adapt their architecture to make efficient use of material under varying functional influences. The architecture of bone arises principally from the information contained within the bone cells’ genetic program [1], and a variety of systemic factors, including hormonal [2] and dietary [3] considerations, as well as site-specific factors, such as the local mechanical environment (cf., [4] and [5]). The ability of exogenous mechanical loading to elicit an adaptive response has received much attention with the aim of developing non-pharmacological interventions to mitigate bone structure deterioration related to aging, osteoporosis, long-term bed rest, and spaceflight.

Although it is agreed that interstitial bone fluid serves as a coupling medium through which external mechanical signals can be transduced into a cellular response – a process termed mechanocoupling [6] – the precise stimulatory signal, or
combination thereof, remains incompletely understood.

Dynamic loading elicits changes in bone fluid pressure, fluid flow through bone’s microchannels (i.e., lacunocanaliculair network), enhanced chemotransport, and electrical potentials from the flow of charged particles, each of which has been suggested to provide the cellular stimulation necessary for functional adaptation (cf., [7 – [10]).

It is inherently difficult to study in situ bone fluid flow. The mineralized nature of bone and the small scale of the pore spaces (0.1 – 100 μm [11]) preclude direct measurement of intrinsic fluid characteristics. As an alternative, investigators have employed the theory of poroelasticity to gain an enhanced understanding of the role of extracellular fluid flow in mechanocoupling.

The theory of poroelasticity was proposed by Biot [12], later refined by Rice and Cleary [13], as a theoretical extension of soil consolidation models developed to calculate the settlement of structures placed on fluid-saturated porous soils [14]. It is a mathematically sophisticated theory that models the influence of solid deformation on fluid flow (and vice versa) (see Appendix for derivation of poroelastic field equations).

A load applied to a block of fluid-saturated porous elastic material will be carried partly by the solid and partly by the fluid. As the fluid is forced from the pores, the solid material will carry an increasing portion of the load. The mechanical behaviour is, therefore, governed both by the elastic deformation of the solid and the flow of fluid in the pores. In essence, poroelasticity replaces the biphasic fluid-saturated solid with a single-phase material whose behaviour matches that of the two phases acting in concert.

The theory was first applied to bone by Nowinski and Davis [15] in a model of the human skull. In their study, the mathematical aspect of the problem was facilitated by applying several key assumptions. (1) The volume distribution of pores in the bulk material is uniform, rendering the material “quasi-isotropic”. (2) Inertial effects are disregarded (small in reality). (3) The solid phase is linearly elastic and undergoes small deformations; its mechanical behaviour is therefore governed by Hooke’s law. The liquid phase is considered Newtonian, whereby the fluid’s stress state is linearly proportional to its strain state (the proportionality constant is the fluid viscosity). (4) The pores form a single contiguous fluid space. (5) The bulk flow of fluid, produced by deformation of the solid, is governed by Darcy’s law, which states that fluid velocity is a function of the pressure drop across a given distance, and a proportionality constant (solid phase permeability divided by fluid viscosity) (see (A.1)).

The oil industry, in its efforts to extract unrefined petroleum from subsurface reservoirs, has a long history of development of simulators capable of modeling geotechnical problems. Conventional reservoir simulators are highly evolved in the treatment of multi-phase flow and heat transfer in porous media. However, conventional simulators typically employ an empirical relation for solid deformation (i.e., change in porosity) and pressure, and are therefore insufficient to explain a wide variety of reservoir phenomena that occur during production, such as subsidence, compaction, casing damage, wellbore stability, and sand production [16]. The physical impact from these geomechanical aspects of reservoir behaviour led to the recent development of coupled simulators that model solid and fluid interactions with the theory of poroelasticity.

Bone fluid flow exhibits several important commonalities with that of fluid flow in geotechnical applications. Specifically, in both instances, fluid flow is pressure-driven; diffusive processes, multi-scale and multi-component flow characteristics, and poromechanical behaviour are present; and both can be influenced by biochemical processes.

A. Methods of Fluid-Solid Coupling

Numerical modeling of geotechnical fluid/solid coupling is complex and has historically been performed in two separate areas: geomechanical modeling (computes stress and strain) and reservoir simulation (models multiphase flow and heat transfer in porous media) [17]. Each discipline makes simplifying assumptions about the part of the problem that is not of primary interest. For example, conventional reservoir simulators generally represent the porosity change of the solid by a simple function of pressure, or may use a pressure-dependent compressibility $c_i = c_i(p)$ to approximate geomechanical effects. These treatments of fluid/solid interactions can generally be classified as pseudocoupling and explicit coupling, respectively [16].

In pseudocoupling, the porosity of the medium is computed from an empirical model, which is implemented in the reservoir simulator. The computer runtime is normally small since there is no need to use a mechanics module. This method provides rough estimations and can be useful to approximate solutions without rigorous mechanics calculations.

Explicit coupling is sometimes called a one-way coupling method because the information is transferred only from the reservoir simulator to the mechanics module. Consequently, changes in the pore pressure field induce changes in stresses and strains, but changes in the stress and strain fields do not affect pore pressures. This method is useful only when the mass balance is mainly controlled by pressure rather than by the stresses of the solid.

The pseudocoupling and explicit coupling methods are insufficient where there is strong interaction among the fluid and solid phases, and particularly where the solid stress largely influences the pore pressure, as is the case in bone fluid flow problems. In these cases more sophisticated approaches, such as full coupling or iterative coupling of
stress and flow are necessary.

In full coupling, the flow variables (i.e., pressure) and mechanical response (i.e., displacement) are calculated simultaneously through a system of equations with pressure and displacements as unknowns. The method is sometimes referred to as implicit coupling because the whole system is discretized on one grid domain and solved simultaneously. Full coupling typically gives good solutions, but is generally less stable numerically, and the extensive computer runtime is a significant disadvantage, particularly for large models.

In iterative coupling, reservoir flow variables and mechanics variables are solved separately and sequentially by a reservoir simulator and a mechanics module, and the coupling terms are iterated at each timestep. The coupling iteration is controlled by a convergence criterion that is normally based on pressure or stress changes between the last two iterates of the solution. This method is more flexible and convenient, since one mechanics module can be coupled with any reservoir simulator without substantial code modifications. If convergence of the coupling iteration is achieved, the solution can be comparable to a fully coupled solution. A further advantage of iterative coupling is the ability to simulate multi-component flow, which allows for investigation of a wide-range of problems beyond simple fluid flow (e.g., nutrient transport; cf., [18]).

B. STARS: Steam, Thermal, and Advanced Process Simulator

STARS is a coupled fluid flow and geomechanics simulator developed by Computer Modelling Group Ltd. (Calgary, AB, Canada) and used extensively by the petroleum industry worldwide. The fluid flow model [19], [20] is a multi-phase, multi-component reactive flow module that can simulate the injection and flow of gases, solvents, polymers, surfactants, and other chemicals. It can be run isothermally or model thermal processes and effects, and includes electrical resistive heating capabilities. The geomechanics module can model linear and nonlinear elasticity, elasto-plastic and visco-elastic behaviour, and fracturing effects.

Fluid/solid coupling in STARS is performed by way of a novel iterative coupling scheme. Through the technique of iterative coupling, information is exchanged between a reservoir simulator and a mechanics module. The mechanics module obtains pressure from the reservoir simulator and treats this information as an external load in the calculation of displacements. When displacements are computed, strains and stresses are determined through the strain-displacement and stress-strain relations, respectively. After the mechanics solution is obtained, compressibility factors for a specialized porosity function are calculated and sent to the coupling driver. Based on the updated porosity function, the pressure is computed in the reservoir simulator and sent back to the mechanics module. The process of coupling is repeated until convergence is achieved (i.e., when the norm of pressure or stress change between two consecutive coupling iterations is below a given tolerance). The process of iterative coupling is illustrated in Fig. 1.

The essence of the iterative coupling method is the use of a specialized porosity function in the simulator, such that porosity is expressed in terms of pressure and mean total stress:

$$\phi^* = \phi^*(p, \sigma_m),$$

(1)

with $\phi^*$ defined as the reservoir porosity, given by

$$\phi^* = \frac{V_p}{V_b},$$

(2)

The reservoir porosity $\phi^*$ is related to the true porosity,

$$\phi = \frac{V_p}{V_b},$$

(3)

by

$$\phi^* = \phi(1 - \varepsilon_r),$$

(4)

where

$$\varepsilon_r = 1 - \frac{V_{b, n}}{V_{b, n+1}}.$$  

(5)

The reservoir simulator performs fluid flow calculations on a fixed grid, whereas the mechanics calculations are performed on a deformable grid. Consequently, the reservoir porosity $\phi^*$ acts as an “effective porosity” in the reservoir simulator that indirectly accounts for the deformation of the grid.

Expansion of (1) as a Taylor’s series between time step $n$ and $n+1$ yields

$$\phi^{n+1} = \phi^n + \left( \frac{\partial \phi^*}{\partial p} \right) \Delta p + \left( \frac{\partial \phi^*}{\partial \sigma_m} \right) \Delta \sigma_m + O^2(p, \sigma_m),$$

(6)

where $\Delta p$ and $\Delta \sigma_m$ are the changes in pressure and mean total stress from step $n$ to $n+1$. Following substitution for the partial derivatives and manipulations (see [16]), (6) can be written as

$$\phi^{n+1} = \phi^n + c_p \Delta p + c_\sigma \Delta \sigma_m,$$

(7)

where $c_p$ and $c_\sigma$ are effective compressibility coefficients that are updated during each coupling iteration, given by

$$c_p = \frac{\left( 1 + \varepsilon_r^* \right)}{K_d} \left( \frac{\left( 1 + \phi^* - \varepsilon_r^* - \phi^* \varepsilon_r^* \right)}{K_s} \right),$$

(8)

and

$$c_\sigma = \frac{\left( 1 - \varepsilon_r^* \right)}{K_d} + \frac{\left( 1 - \varepsilon_r^* \right)}{K_s}.$$  

(9)
II. EXAMPLE PROBLEMS

In the following example problems the applicability of the STARS reservoir simulator to the solution of problems in bone fluid flow is demonstrated. Firstly, the iteratively coupled scheme is validated against the analytical solution of a well-known geomechanical problem. Secondly, computational results of a bone specimen under cyclical loading are compared to a previous numerical study. Lastly, a dual-material example is elaborated to illustrate the potential for modeling the multiple levels of porosity present in bone.

The geometry of the model was based on the poroelastic prismatic solid examined by Zhang and Cowin [21] (Fig. 2).

![Schematic of poroelastic solid.](image)

The model dimensions used for the example problems are listed in table I.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Examples A and B</th>
<th>Example C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>2.5 mm</td>
<td>0.25 mm</td>
</tr>
<tr>
<td>$b$</td>
<td>0.5 mm</td>
<td>0.05 mm</td>
</tr>
<tr>
<td>$w$</td>
<td>0.5 mm</td>
<td>0.05 mm</td>
</tr>
</tbody>
</table>

The boundary conditions imposed on the solid were modified for each example and are described in their respective sections.

A. Mandel-Cryer Effect

As a verification of the iterative coupling technique, the classical Mandel problem with the experimentally confirmed Mandel-Cryer effect [22], [23] was recreated.

Mandel's problem involves an infinitely wide ($w \to \infty$) rectangular specimen constrained at the top and bottom ($z = \pm b$) by two rigid, frictionless, and impermeable plates. The lateral boundaries ($x = \pm a$) are free of normal and shear stresses, and are exposed to the ambient pressure, equivalent to the initial pore pressure $p^o$. At $t = 0^+$ a step-load of $2N_0$ is applied to the rigid plates.

The two-dimensional problem is solved numerically using STARS' three-dimensional model by imposing a plane strain condition (i.e., $u_z = 0$). Symmetry about the $x-$ and $z-$axes allowed the computational domain to be reduced to a quarter of the specimen size (Fig. 3). The rigid plate condition was enforced by restricting all nodes on the top surface ($z = b$) to move with uniform displacement $u_z$.

![Schematic of computational domain for Mandel-Cryer problem.](image)

The computational domain was discretized into 500 ($50 \times 1 \times 10$) 8-noded hexahedral elements, each measuring $50 \times 50 \times 50 \mu m$.

The specimen consisted of an incompressible solid constituent and was saturated with an incompressible fluid. In this special case, $K_s$ and $K_f > K_h$, and from (A.13) and (A.14), $a = 1$ and $B = 1$.

From Rice and Cleary [13], the undrained Poisson’s ratio may be defined as

$$v = \frac{3v_f + \alpha B (1 - 2v_f)}{3 - \alpha B (1 - 2v_f)}.$$  \hspace{1cm} (10)

The parameters and material properties used in the calculations are summarized in table II.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_0$</td>
<td>2.5 kN</td>
<td>$a$</td>
<td>1.0</td>
</tr>
<tr>
<td>$p^o$</td>
<td>0.0 Pa</td>
<td>$B$</td>
<td>1.0</td>
</tr>
<tr>
<td>$E_d$</td>
<td>18 GPa</td>
<td>$k$</td>
<td>$10^{-20}$ m$^2$</td>
</tr>
<tr>
<td>$v_u$</td>
<td>0.5</td>
<td>$\phi$</td>
<td>0.05</td>
</tr>
<tr>
<td>$v_d$</td>
<td>0.25</td>
<td>$1/K_f$</td>
<td>0.0 GPa$^{1/3}$</td>
</tr>
</tbody>
</table>

![Table II. Mandel-Cryer parameter values.](image)
Abousleiman et al. [23] extended Mandel’s original solution [22] for the pore pressure to all field quantities. Their analytical solutions were given as follows:

\[
\begin{align*}
    u_x &= \left[ \frac{N_v v_x}{2G_d a} + \sum_{\mu=1}^{\infty} \frac{\sin \beta_i \cos \beta_i}{\mu \beta_i - \sin \beta_i \cos \beta_i} \exp \left( -\frac{\beta_i^2 c t}{a^2} \right) \right] \times \left[ \frac{N_v}{G_d a} \sum_{\mu=1}^{\infty} \frac{\cos \beta_i}{\mu \beta_i - \sin \beta_i \cos \beta_i} \exp \left( -\frac{\beta_i^2 c t}{a^2} \right) \right] + \frac{N_v}{G_d a} \sum_{\mu=1}^{\infty} \frac{\cos \beta_i x}{\mu \beta_i - \sin \beta_i \cos \beta_i} \exp \left( -\frac{\beta_i^2 c t}{a^2} \right), \\
    u_y &= \left[ -\frac{N_v (1 - v_y)}{2G_d a} - \sum_{\mu=1}^{\infty} \frac{\sin \beta_i \cos \beta_i}{\mu \beta_i - \sin \beta_i \cos \beta_i} \exp \left( -\frac{\beta_i^2 c t}{a^2} \right) \right], \\
    p &= \frac{2N_v B (1 + v_y)}{3a} \sum_{\mu=1}^{\infty} \frac{\sin \beta_i \cos \beta_i}{\mu \beta_i - \sin \beta_i \cos \beta_i} \left( \frac{\cos \beta_i x}{a} - \cos \beta_i \right) \exp \left( -\frac{\beta_i^2 c t}{a^2} \right), \\
    \sigma_{zz} &= -\frac{N_v}{a} \frac{2N_v (v_y - v_d)}{a (1 - v_d)} \sum_{\mu=1}^{\infty} \frac{\sin \beta_i \cos \beta_i}{\mu \beta_i - \sin \beta_i \cos \beta_i} \exp \left( -\frac{\beta_i^2 c t}{a^2} \right) + \frac{2N_v}{a} \sum_{\mu=1}^{\infty} \frac{\sin \beta_i \cos \beta_i}{\mu \beta_i - \sin \beta_i \cos \beta_i} \exp \left( -\frac{\beta_i^2 c t}{a^2} \right), \\
    \sigma_{yy} &= \sigma_{zz} = 0, \\
    \beta_i &= \tan \beta_i = \frac{1 - v_d}{v_y - v_d},
\end{align*}
\]

As time progresses, the pressure gradient at the lateral boundary induces drainage, and the pressure depletion region propagates into the center of the specimen \((x = 0)\). The initial presence of pore pressure adds to the apparent stiffness of the material. Thus, as the pressure is reduced at the lateral boundary, the specimen becomes more compliant near the sides [23]. As a result, there is a load transfer toward the centre of the specimen, which serves as a mechanism of pressure generation. Consequently, the pore pressure in the centre region continues to rise after the uniform creation \(\Delta p(x, z, 0^+\) (Fig. 4a). This non-monotonic pore pressure response, referred to as the Mandel-Cryer effect, is a unique phenomenon not observable in general non-coupled free-drainage problems.

Fluid drainage will cease once the pore pressure is dissipated over the entire domain. At this point, the specimen will have stabilized at [25]

\[
\begin{align*}
    u_x(a, z, \infty) &= \frac{N_v v_x}{2G_d}, \\
    u_y(a, z, \infty) &= \frac{N_v b(1 - v_y)}{2G_d a}.
\end{align*}
\]

According to the analytical solution, immediately following load application a uniform pressure rise due to the Skempton effect [24] and instantaneous displacements of the lateral and top surfaces are generated and are given respectively by [25]

\[
\begin{align*}
    \Delta p(x, z, 0^+) &= \frac{N_v B (1 + v_y)}{3a}, \\
    u_x(a, z, 0^+) &= \frac{N_v v_x}{2G_d}, \\
    u_y(a, z, 0^+) &= \frac{N_v b(1 - v_y)}{2G_d a}, \\
    u_y(x, b, 0^+) &= -\frac{N_v b(1 - v_y)}{2G_d a}.
\end{align*}
\]
Figure 4. Comparison of analytical and numerical solutions of Mandel-Cryer problem at selected time steps. (a) Normalized pressure $= \frac{ap}{F}$. (b) Normalized stress $= \sigma_{\text{num}} / F$. (c) Normalized $x$-displacement $= u_x / a$. (d) Normalized $z$-displacement $= u_z / b$.

**B. Cyclic Loading**

In this example, the poroelastic solid was subjected to combined cyclic axial force and bending moment to simulate bone behaviour following the analytical study of Zhang and Cowin [20] and the subsequent numerical analysis by Manfredini et al. [26].

The porous skeleton was composed of a compressible solid constituent and was saturated with a compressible fluid. The top and bottom surfaces of the specimen were exposed to the ambient pressure, equivalent to the initial pore pressure $p^0$, and the pressure gradient across the vertical surfaces ($x = \pm a$; $y = \pm w$) was defined as zero (i.e., impermeable to flow). In view of the symmetries, appropriate boundary conditions were applied to reduce the computational domain to a quarter of the specimen size (Fig. 5): zero $y$–displacement for nodes on the plane of symmetry defined by the $x$– and $z$–axes, and zero $x$–displacement for nodes on the plane of symmetry defined by the $y$– and $z$–axes. Convergence analysis (results not presented) demonstrated solution accuracy for a three-dimensional finite element mesh consisting of 2,500 (25 x 5 x 20) 8-noded hexahedral elements, each measuring $100 \times 100 \times 50 \mu m$.

Figure 5. Schematic of cyclically loaded poroelastic solid. Shaded faces represent planes of symmetry.

The specimen was subjected to cyclic axial loading and bending moment given by

$$N(t) = N_0 \sin(\omega t),$$

and

$$M(t) = M_0 \sin(\omega t),$$

respectively (see Fig. 4). Bending was induced with distributed point loads applied at the unconstrained end of the specimen ($x = a$, $z = 0$). The magnitude of the point loads was selected to produce a moment equivalent to $M(t)$ about the $y$–axis. To implement the bending loads, an additional constraint was required whereby the nodes on the plane of symmetry defined by the $y$– and $z$–axes were constrained to zero displacement in the $z$–direction.
Manfredini et al. [26] used the material parameters $G_d$, $\alpha$, $v_d$, and $v_u$, from which we calculated $E_d$, $K_d$, and $B$ using (A.11), (A.12), and (A.14), respectively. The porosity $\phi$ was taken to be that associated with the lacunocanalicular fluid space [21].

The parameter values and material properties used in the calculations are listed in Table IV.

**Table IV. Poroelastic specimen parameter values for cyclic loading example.**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_0$</td>
<td>1 N</td>
<td>$\alpha$</td>
<td>0.25</td>
</tr>
<tr>
<td>$p^o$</td>
<td>0.0 Pa</td>
<td>$B$</td>
<td>0.53</td>
</tr>
<tr>
<td>$E_d$</td>
<td>18 GPa</td>
<td>$k$</td>
<td>$10^{-20}$ m$^2$</td>
</tr>
<tr>
<td>$v_d$</td>
<td>0.28</td>
<td>$\phi$</td>
<td>0.05</td>
</tr>
<tr>
<td>$v_u$</td>
<td>0.25</td>
<td>$K_f$</td>
<td>2.3 GPa</td>
</tr>
</tbody>
</table>

Six simulations were performed varying two nondimensional parameters: the dimensionless frequency $T$, and the dimensionless bending moment $m$, defined as

$$T = \frac{\omega b^2}{c},$$

and

$$m = \frac{3M_0}{N_0 b},$$

where

$$c = \frac{k}{\mu} \frac{2G_d(1-v_d)(1-v_u)}{\alpha^2(1-2v_d)(1-v_u) \left[ 1 - \frac{E_d}{E_u} \right]^{1/2}} [27].$$

The value of $T$ was varied by changing the permeability $k$ in the diffusion coefficient $c$, while $m$ was varied by changing the magnitude of the bending moment $M_0$ (i.e., in the present study, the magnitude of the bending loads).

Figs. 6 and 7 present the pore pressure time series and pressure distribution across the thickness ($2b$) of the poroelastic solid. Following previous studies [21], [26], the pore pressure was calculated in nondimensional form, given by

$$P(t, Z) = \frac{2\psi b}{N_0} \psi^2 - p(t, Z),$$

where

$$\psi = \frac{\alpha(1-2v_d)(1+v_d)(1-v_u)}{(v_d-v_u)(1-v_u)}$$

and

$$\tau = \frac{ct}{b^2}. $$

The free-drainage condition imposed on the top and bottom surfaces ($Z = 1.0, -1.0$) maintained the pressure at these two surfaces at zero. Consistent with the analytical solution, the magnitude of the pressure increased as $T$ increased in value (Fig. 6), and the pressure profile across the thickness $Z$ transformed from a parabolic shape to a linear shape (cf. Fig. 5; [21]). As $m$ was increased from 0.1, 10, to 100 (Fig. 7), $P$ increased dramatically, and the profile changed from a symmetric shape about $Z = 0$ to an antisymmetric S-shape about $Z = 0$ (cf. Fig. 6; [21]).

For all cases considered here, the calculated pressure distribution across the thickness exhibited a high degree of similarity to the curves produced by Manfredini et al. [26] and Zhang and Cowin [21]. However, the pressure magnitudes for the six cases in the present study were approximately 1.57–times smaller than those reported previously. This was attributed to the modified boundary conditions employed to simulate the bending moment.
Figure 6. Pore pressure ($P$) distribution throughout the poroelastic solid thickness $Z(x = 0; y = 0)$ for $m = 1.0$ and (a) $T = 0.1$, (b) $T = 10$, and (c) $T = 100$. Above, the pressure and loading time series are presented ($x = 0; y = w/2; z = h$), and dimensionless time-points used for pressure distribution are illustrated by broken vertical lines.

Figure 7. Pore pressure ($P$) distribution throughout the poroelastic solid thickness $Z(x = 0; y = 0)$ for $T = 1.0$ and (a) $m = 0.1$, (b) $m = 10$, and (c) $m = 100$. Above, the pressure and loading time series are presented ($x = 0; y = w/2; z = h$), and dimensionless time-points used for pressure distribution are illustrated (broken vertical lines).
C. Dual-Continuum Model

The bulk of the diaphyseal cortex in mature humans is comprised of secondary osteons [28], which are the basic structural unit of cortical bone, measuring ~250 μm in diameter [11]. The osteon has three hierarchically arranged levels of porosity, each containing a fluid phase [14]. In order of decreasing characteristic linear dimension, they are: the vascular porosity, the lacunocanicular porosity, and the collagen-apatite porosity. The vascular and lacunocanicular porosities are intimately linked in regards to fluid exchange; however, it is not clear if the collagen-apatite porosity contributes to the contiguous fluid space in bone.

The vascular porosity is believed to act as a mechanism for the dissipation of lacunocanicular pore fluid pressure generated during mechanical loading [29] and is an important source for cellular nourishment [30]. Consequently, the multi-porosity nature of bone represents a significant aspect of its structure that influences its mechanical response and biological processes.

In this example, the poroelastic solid is modified to illustrate the capability of STARS, with the iterative coupling scheme, to simulate the mechanical behaviour of a dual-continuum specimen at a smaller bone scale (e.g., osteonal scale) (see table I).

A block of dimensions \( a \times b \times w \) was inserted in the centre of the poroelastic solid. In light of the three planes of symmetry, appropriate boundary conditions allowed the computational domain to be reduced to a quarter of the entire specimen (Fig. 8): zero-displacement in the \( x \)-direction for nodes on the plane defined by the \( y \)- and \( z \)-axes; zero-displacement in the \( y \)-direction for nodes on the plane defined by the \( x \)- and \( y \)-axes; and zero-displacement in the \( z \)-direction for nodes on the plane defined by the \( x \)- and \( y \)-axes. The computational domain for the three-dimensional poroelastic solid was discretized into 5,000 elements \((50 \times 10 \times 10)\), each measuring \( 5 \times 5 \times 5 \) μm.

The outer block was assigned properties representative of the lacunocanicular porosity [31], while the inner block was assigned properties of a more porous and permeable material (table V).

<table>
<thead>
<tr>
<th>Property</th>
<th>Outer Material</th>
<th>Inner Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_d )</td>
<td>18 GPa</td>
<td>1.8 GPa</td>
</tr>
<tr>
<td>( \nu_d )</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>( a )</td>
<td>0.25</td>
<td>1.0</td>
</tr>
<tr>
<td>( B )</td>
<td>0.53</td>
<td>1.0</td>
</tr>
<tr>
<td>( k )</td>
<td>( 10^{-20} ) m(^2)</td>
<td>( 10^{-18} ) m(^2)</td>
</tr>
<tr>
<td>( \phi )</td>
<td>0.05</td>
<td>0.20</td>
</tr>
<tr>
<td>( K_f )</td>
<td>2.3 GPa</td>
<td>2.3 GPa</td>
</tr>
</tbody>
</table>

The outer block was impermeable with respect to the surrounding environment (i.e., no mass transport) to highlight the fluid exchange between the two materials. At \( t = 0^+ \) a distributed step-load (stress) \( N_0 \) of 10 MPa was applied to the top surface of the outer block, and the initial and transient responses of the specimen were calculated. In this case, the top surface was not constrained to move as a rigid body, as in Example 4.

Immediately following application of the distributed load, a maximal compressive volumetric strain of 1,188 με was calculated in the inner material at \( z = \frac{1}{2} b \) (Fig. 9a). The inner and outer materials exhibited average volumetric strains of 640 and 260 με, respectively. A region of decreased strain and volumetric expansion of ~338 με was produced in the outer material directly above the inner material.

Volumetric strain induced pore fluid pressure in the inner and outer materials (Fig. 9b). The large deformation of the more compliant inner material resulted in greater pore pressure in the core than in the stiff outer material. A maximal pore pressure rise of 1,887 kPa was calculated in the inner material at \( z = \frac{1}{2} b \). Average pressures of 1,400 and 119 kPa were calculated in the inner and outer materials, respectively. Similar pressure magnitudes have been previously calculated in the lacunocanicular porosity (cf., [32]).

The non-monotonic pressure rise in the specimen produced fluid flow in the pore spaces in accordance with Darcy’s law (A.1) (Fig. 9c). Maximal fluid velocity was calculated in the core at a magnitude of 29.3 μm s\(^{-1}\). Load-induced pressure forced fluid from the high-pressure core to the low-pressure outer material (Fig. 10).

Transfer of fluid mass from the inner to the outer material served to relax the pore pressure generated in the soft core, while increasing the pore pressure in the stiff outer material (Fig. 11). Approximately 170 μs after loading, the entire poroelastic specimen was equilibrated in pressure at 815 kPa.
increased \((t_\text{f} = 5)\). After 167 \(\mu\text{s}\), a uniform pressure in the poroelastic specimen was calculated \((\delta_\text{f})\).

### III. Conclusion

In this study, a method for coupling fluid flow and mechanical deformation was presented. The iteratively coupled scheme of the STARS reservoir simulator was then applied to three example problems illustrating: (1) the Mandel-Cryer phenomenon, (2) a bone specimen under cyclical loading, (3) and a dual-continuum bone specimen. Through these examples, model validity and accuracy of the numerical scheme were verified, and the utility of STARS as a sophisticated tool for the study of problems in bone fluid flow was demonstrated.

As it remains inherently difficult to study bone fluid flow experimentally, the ability to simulate accurately the fluid-mechanical interactions in bone at various length scales and with multiple material (continuum) models represents an important alternative to experimental investigation. Advanced theoretical studies based on the models developed here will provide an enhanced understanding of the role of extracellular fluid flow in functional adaptation of bone, as well as offer insights into potential experimental techniques.

### Appendix

#### Poroelastic Field Equations

Fluid motions in porous media are governed by the same fundamental laws that govern their motion in other environments, such as the atmosphere, pipelines, and rivers. These laws are based on the conservation of mass, momentum, and energy. Practically, it is overly complex to apply these laws directly to the problems of flow in porous media. Alternatively, a semi-empirical approach is used where Darcy’s law is employed instead of the momentum equation. Moreover, as we are concerned with isothermal processes (body temperature of 37 °C), an energy balance is not required.

Darcy’s law is a phenomenologically derived constitutive equation that describes the relation between the flow rate and pressure gradient in a porous medium. It is a form of the balance of linear momentum. In compact differential form, Darcy’s law for three-dimensional single-component flow can be expressed as:

\[
\mathbf{q} = -\frac{k}{\mu} \nabla p. \tag{A.1}
\]

In addition to Darcy’s law, it is necessary to specify porosity and an equation of state for the fluid (i.e., constitutive relations between porosity, density and pressure) [33]: \(\phi = \phi(p)\) and \(\rho = \rho(p)\). In a conventional reservoir simulator (no solid deformation), if the variation of pore volume with pressure is significant, it may be accounted for by
\[ \phi = \phi \left[ 1 + \frac{1}{K_f} (p - p^*) \right]. \]  
\[ (A.2) \]

Similarly, the variation of fluid density with pressure is given by
\[ \rho = \rho \left[ 1 + \frac{1}{K_f} (p - p^*) \right]. \]  
\[ (A.3) \]

The differential equation for fluid flow is obtained by combining the constitutive equations (A.1), (A.2), and (A.3) with a material balance, derived from the law of mass conservation for three-dimensional single-component flow in a porous medium of arbitrary shape:
\[ \nabla \cdot (\rho \mathbf{q}) = \frac{\partial (\rho \phi)}{\partial t} + \Omega, \]  
\[ (A.4) \]

where \( \Omega \) is the rate of injection/production (mass per unit volume per unit time).

The behaviour of the fluid constituent may therefore be described in terms of the pressure by
\[ \nabla \cdot (c \nabla p) = \frac{\partial \rho}{\partial t} + \Omega', \]  
\[ (A.5) \]

with
\[ c = \frac{k K_f \rho}{\mu (K_f \phi^* + K_f \phi^* \rho)}, \]  
\[ (A.6) \]

where \( c \) has units of length squared per time, which dictates how fluid pressure in the system relaxes over time.

The constitutive response for the solid skeleton is represented by the isotropic stress-strain relations,
\[ \sigma_{ij} + \alpha p \delta_{ij} = 2G_{ij} \varepsilon_{ij} + \frac{2G_d \nu_d}{1 - 2\nu_d} \sum_{k=1}^{3} \varepsilon_{kk} \delta_{ij}, \]  
\[ (A.7) \]

where \( \alpha \) is the ratio of the fluid volume gained or lost in a material element due to the volume change of that element when loaded under the drained condition (also referred to as Biot’s coefficient), and \( \delta_{ij} \) is defined as 1 when its indices agree and 0 otherwise. The constitutive equations are similar to that for a purely elastic solid with \( (\sigma_{ij} + \alpha p \delta_{ij}) \) acting as an “effective stress,” and thus, the coefficient \( \alpha \) is also interpreted as an effective stress coefficient.

The field equations for the solid constituent are obtained through combination of the constitutive relations and the conservation of linear momentum for the solid phase, employed in the form of the stress equations of equilibrium,
\[ \sum_{i=1}^{3} \frac{\partial \sigma_{ij}}{\partial x_i} = -b_j, \]  
\[ (A.8) \]
where \( b_j \) is the body force per unit volume of the bulk material.

The mechanical behaviour of a solid may therefore be described in terms of the solid displacement vector \( u_i \) by substituting the constitutive relation, (A.7), into the equilibrium equation (A.8), with \( \varepsilon_{ij} \) expressed in terms of the displacement gradient,
\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \]  
\[ (A.9) \]
\[ G_j \nabla^2 u_i + \frac{G_d}{1 - 2\nu_d} \frac{\partial}{\partial x_j} \left( \sum_{j=1}^{3} \frac{\partial u_i}{\partial x_j} \right) = dV \rho - b_j. \]  
\[ (A.10) \]

A set of four material constants is required to characterize a linear isotropic poroelastic material. For example, with the addition of the following relations [27]
\[ G_d = \frac{E_d}{2(1 + \nu_d)}, \]  
\[ (A.11) \]
\[ K_d = \frac{2G (1 + \nu_d)}{\chi (1 - 2\nu_d)}, \]  
\[ (A.12) \]
\[ \alpha = 1 - \frac{K_d}{K_s}, \]  
\[ (A.13) \]
\[ B = \frac{\alpha K_f}{[\alpha - \phi (1 - \alpha) K_f] + \phi K_d}, \]  
\[ (A.14) \]
the mechanical behaviour of a fluid-saturated medium may be described by \( E_d, \nu_d, B, \) and \( \alpha \). Skempton’s coefficient \( B \) is a measure of the relative compressibilities (\( 1/K \)) of the fluid and solid phases and determines the proportion of the mean stress that is “carried” by the pore fluid. By specifying the mechanical constants, the porosity \( \phi \) of the medium, and the hydraulic properties – permeability \( k \) and dynamic fluid viscosity \( \mu \) – a complete poroelastic formulation is obtained.

**REFERENCES**