GRES: Report

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1 Mathematical models

1.1 Single-phase slightly compressible flow in porous media

$$\nabla \cdot \boldsymbol{v} = -\sigma \frac{\partial p}{\partial t} - q \tag{1}$$

where:

- $\sigma = \alpha + \phi\beta$ is the storage coefficient [1/P];
- ϕ is porosity [/];
- $\alpha = d\phi/dp$ is the rock compressibility [1/P];
- $\beta = (1/\rho)(d\rho/dp)$ is the fluid compressibility [1/P] with ρ being its density;
- q is the source/sink, i.e., the volumetric fluid flow injected or produced [1/T].

$\boldsymbol{v}$ is Darcy's velocity

$$\boldsymbol{v} = -\frac{K}{\mu}\nabla(p + \gamma z) \tag{2}$$

where:

- K is the permeability matrix [L^3];
- μ is the dynamic viscosity [P$\times$T].

The flow equation:

$$\nabla \cdot \left[\frac{K}{\mu}\nabla\left(p + \gamma z\right)\right] = \sigma \frac{\partial p}{\partial t} + q \tag{3}$$

The flow equation is *linear*. The parameter α in σ is replaced by the odometer compressibility C_M derived from the poromechanical properties of the rock and the specific constitutive law.

2 Numerical models

2.1 Single-phase slightly compressible flow in porous media

We use the FE method.

$$p \approx \hat{p}(x,y,z,t) = \sum_{i=1}^{n} p_i(t)\xi_i(x,y,z) \tag{4}$$

$$L(\hat{p}) = \nabla \cdot \left[\frac{K}{\mu}\nabla\left(\hat{p}+\gamma z\right)\right] - \sigma\frac{\partial \hat{p}}{\partial t} - q \tag{5}$$

$$\int_\Omega L(\hat{p})\xi_i \, d\Omega = 0 \qquad i = 1,\ldots,n \tag{6}$$

$$\int_\Omega \nabla \cdot \boldsymbol{\Gamma}\psi d\Omega = \int_{\partial\Omega} (\boldsymbol{\Gamma}\cdot\boldsymbol{n})\psi ds - \int_\Omega \nabla\psi \cdot \boldsymbol{\Gamma} d\Omega \tag{7}$$

$$\begin{aligned} -\int_\Omega \nabla{\xi_i}^T \left[\frac{K}{\mu}\nabla\left(\hat{p}+\gamma z\right)\right] d\Omega + \int_\Gamma \left[\frac{K}{\mu}\nabla(p+\gamma z)\cdot\boldsymbol{n}\right]\xi_i \, d\Gamma \\ - \int_\Omega \sigma\frac{\partial \hat{p}}{\partial t}\xi_i \, d\Omega - \int_\Omega q\xi_i \, d\Omega = 0 \qquad i = 1,\ldots,n \end{aligned} \tag{8}$$

$$\frac{K}{\mu}\nabla(p+\gamma z)\cdot\boldsymbol{n} = q_n \tag{9}$$

$$\begin{aligned} \int_\Omega \nabla{\xi_i}^T\frac{K}{\mu}\nabla\hat{p}\, d\Omega + \int_\Omega \sigma\frac{\partial\hat{p}}{\partial t}\xi_i \, d\Omega + \int_\Omega \nabla{\xi_i}^T\frac{K}{\mu}\gamma\nabla z \, d\Omega \\ + \int_\Omega q\xi_i \, d\Omega - \int_{\Gamma_q} q_n\xi_i \, d\Gamma = 0 \qquad i = 1,\ldots,n \end{aligned} \tag{10}$$

$$\begin{aligned} \int_\Omega \left(\sum_{j=1}^{n} \nabla{\xi_i}^T\frac{K}{\mu}\nabla\xi_j p_j\right) d\Omega + \int_\Omega \left(\sum_{j=1}^{n}\sigma\xi_i\xi_j\frac{\partial p_j}{\partial t}\right) d\Omega \\ + \int_\Omega \nabla{\xi_i}^T\frac{K}{\mu}\gamma\nabla z \, d\Omega + \int_\Omega q\xi_i \, d\Omega - \int_{\Gamma_q} q_n\xi_i \, d\Gamma = 0 \qquad i = 1,\ldots,n \end{aligned} \tag{11}$$

$$H\boldsymbol{p} + P\frac{\partial\boldsymbol{p}}{\partial t} + \boldsymbol{f} = 0 \tag{12}$$

where $\boldsymbol{p} = [p_1, p_2, \ldots, p_l]^T$.

$$H_{ij} = \sum_{e=1}^{l} H_{ij}^e = \sum_{e=1}^{l} \int_{\Omega^e} \nabla \xi_i^{eT} \left(\frac{K}{\mu} \right)^e \nabla \xi_j^e \, d\Omega^e \tag{13}$$

$$P_{ij} = \sum_{e=1}^{l} P_{ij}^e = \sum_{e=1}^{l} \int_{\Omega^e} \sigma^e \xi_i^e \xi_j^e \, d\Omega^e \tag{14}$$

$$f_i = \sum_{e=1}^{l} f_i^e = \sum_{e=1}^{l} \left[\int_{\Omega^e} \nabla \xi_i^{eT} \left(\frac{K}{\mu} \gamma \right)^e \nabla z \, d\Omega^e + \int_{\Omega^e} q^e \xi_i^e \, d\Omega^e - \int_{\Gamma_q^e} q_n^e \xi_i^e \, d\Gamma^e \right] \tag{15}$$

$$\boldsymbol{p}_\tau = \theta \boldsymbol{p}_{t+\Delta t} + (1-\theta) \boldsymbol{p}_t \tag{16}$$

$$\boldsymbol{f}_\tau = \theta \boldsymbol{f}_{t+\Delta t} + (1-\theta) \boldsymbol{f}_t \tag{17}$$

$$\left. \frac{\partial \boldsymbol{p}}{\partial t} \right|_\tau = \frac{\boldsymbol{p}_{t+\Delta t} - \boldsymbol{p}_t}{\Delta t} \tag{18}$$

$$\left(\theta H + \frac{P}{\Delta t} \right) \boldsymbol{p}_{t+\Delta t} = \left[\frac{P}{\Delta t} - (1-\theta) H \right] \boldsymbol{p}_t - \theta \boldsymbol{f}_{t+\Delta t} - (1-\theta) \boldsymbol{f}_t \tag{19}$$

$$K_1 \boldsymbol{p}_{t+\Delta t} = K_2 \boldsymbol{p}_t + \boldsymbol{q} \tag{20}$$

$$K_1 = \theta H + \frac{P}{\Delta t} \tag{21}$$

$$K_2 = \frac{P}{\Delta t} - (1-\theta) H \tag{22}$$

$$\boldsymbol{q} = -\theta \boldsymbol{f}_{t+\Delta t} - (1-\theta) \boldsymbol{f}_t \tag{23}$$

3 FE Matrices

3.1 Tetrahedra

$$\xi_i^e(x, y, z) = a_i + b_i x + c_i y + d_i z \qquad i = 1, \ldots, 4 \tag{24}$$

where

$$\begin{bmatrix} a_1 & a_2 & a_3 & a_4 \\ b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 \\ d_1 & d_2 & d_3 & d_4 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{bmatrix}^{-1} \tag{25}$$

3.2 Hexahedra

An isoparametric map Ψ performs a change of coordinates so that a point $\boldsymbol{x} \in e$ is transformed into a single point $\hat{\boldsymbol{x}} \in \hat{e}$, in symbols:

$$\begin{aligned} \Psi : \mathbb{R}^3 &\longrightarrow \mathbb{R}^3 \\ \hat{\boldsymbol{x}} \in \hat{e} &\longmapsto \boldsymbol{x} = \Psi\left(\hat{\boldsymbol{x}}\right) \in e. \end{aligned} \tag{26}$$

We can express the isoparametric map Ψ with the aid of the FEM basis functions. For the reference hexahedron, these functions read:

$$\xi_i(\hat{x}, \hat{y}, \hat{z}) = \frac{1}{8}(1 + \hat{x}\hat{x}_i)(1 + \hat{y}\hat{y}_i)(1 + \hat{z}\hat{z}_i) \qquad i = 1, \dots, 8 \tag{27}$$

where ξ_i is the basis function of the i-th node and $\hat{x}_i$, $\hat{y}_i$, $\hat{z}_i$ are the coordinates of node i of the reference hexahedron, implying that $\hat{x}_i, \hat{y}_i, \hat{z}_i = \pm 1$ for $i = 1, \dots, 8$. Using eqs. (27), ψ is simply given by:

$$\boldsymbol{x} = \Psi\left(\hat{\boldsymbol{x}}\right) = \begin{bmatrix} x_1 & x_2 & \dots & x_8 \\ y_1 & y_2 & \dots & y_8 \\ z_1 & z_2 & \dots & z_8 \end{bmatrix} \begin{bmatrix} \xi_1\left(\hat{\boldsymbol{x}}\right) \\ \xi_2\left(\hat{\boldsymbol{x}}\right) \\ \vdots \\ \xi_8\left(\hat{\boldsymbol{x}}\right) \end{bmatrix} = X \boldsymbol{\xi}\left(\hat{\boldsymbol{x}}\right), \tag{28}$$

We can express the derivatives of the element basis functions in the physical space in terms of those defined in the reference space as follows:

$$\begin{bmatrix} \frac{\partial \xi_i}{\partial x} \\ \frac{\partial \xi_i}{\partial y} \\ \frac{\partial \xi_i}{\partial z} \end{bmatrix} = J_\Psi^{-1} \begin{bmatrix} \frac{\partial \xi_i}{\partial \hat{x}} \\ \frac{\partial \xi_i}{\partial \hat{y}} \\ \frac{\partial \xi_i}{\partial \hat{z}} \end{bmatrix} \tag{29}$$

Here, J is the Jacobian of the isoparametric transformation:

$$J_\Psi = \begin{bmatrix} \frac{\partial \xi_1(\hat{\boldsymbol{x}})}{\partial \hat{x}} & \frac{\partial \xi_2(\hat{\boldsymbol{x}})}{\partial \hat{x}} & \dots & \frac{\partial \xi_8(\hat{\boldsymbol{x}})}{\partial \hat{x}} \\ \frac{\partial \xi_1(\hat{\boldsymbol{x}})}{\partial \hat{y}} & \frac{\partial \xi_2(\hat{\boldsymbol{x}})}{\partial \hat{y}} & \dots & \frac{\partial \xi_8(\hat{\boldsymbol{x}})}{\partial \hat{y}} \\ \frac{\partial \xi_1(\hat{\boldsymbol{x}})}{\partial \hat{z}} & \frac{\partial \xi_2(\hat{\boldsymbol{x}})}{\partial \hat{z}} & \dots & \frac{\partial \xi_8(\hat{\boldsymbol{x}})}{\partial \hat{z}} \end{bmatrix} \begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ \vdots & \vdots & \vdots \\ x_8 & y_8 & z_8 \end{bmatrix} = J_\xi\left(\hat{\boldsymbol{x}}\right) X \tag{30}$$

Integrals in eqs. (13), (14) and (15) are evaluated numerically with the aid of Gaussian quadrature. Therefore, the Jacobian matrix J_ξ can be computed on each Gauss point once and stored in memory. We obtain a 3-dimensional matrix, denoted in the code as `J1`, where each page refers to a Gauss point. The Jacobian matrix J_Ψ in the code is this expressed as a $3 \times 3 \times nG$ 3-dimensional matrix, `J`. Denoting $\frac{\partial \xi_i^\ell}{\partial \hat{x}}$, $\frac{\partial \xi_i^\ell}{\partial \hat{y}}$, and $\frac{\partial \xi_i^\ell}{\partial \hat{z}}$ as b_i, c_i and d_i, respectively, with $\boldsymbol{x}_\ell$ the location of the ℓ-th Gauss point, the derivatives of the element basis functions in the physical space are simply given by:

$$\begin{bmatrix} b_1 & b_2 & \cdots & b_8 \\ c_1 & c_2 & \cdots & c_8 \\ d_1 & d_2 & \cdots & d_8 \end{bmatrix}_\ell = \begin{bmatrix} j_{11}^{-1} & j_{12}^{-1} & j_{13}^{-1} \\ j_{21}^{-1} & j_{22}^{-1} & j_{23}^{-1} \\ j_{31}^{-1} & j_{32}^{-1} & j_{33}^{-1} \end{bmatrix}_\ell \begin{bmatrix} \frac{\partial \xi_1}{\partial \hat{x}} & \frac{\partial \xi_2}{\partial \hat{x}} & \cdots & \frac{\partial \xi_8}{\partial \hat{x}} \\ \frac{\partial \xi_1}{\partial \hat{y}} & \frac{\partial \xi_2}{\partial \hat{y}} & \cdots & \frac{\partial \xi_8}{\partial \hat{y}} \\ \frac{\partial \xi_1}{\partial \hat{z}} & \frac{\partial \xi_2}{\partial \hat{z}} & \cdots & \frac{\partial \xi_8}{\partial \hat{z}} \end{bmatrix}_\ell \tag{31}$$

3.3 Flow

3.3.1 Tetrahedra

$$H^e = \int_{\Omega^e} \nabla \xi_i^{eT} \left(\frac{K}{\mu}\right)^e \nabla \xi_j^e \, d\Omega^e, \qquad i,j = 1,\ldots,4 \tag{32}$$

$$H^e = \frac{1}{\mu^e} \begin{bmatrix} b_1 & c_1 & d_1 \\ b_2 & c_2 & d_2 \\ b_3 & c_3 & d_3 \\ b_4 & c_4 & d_4 \end{bmatrix} \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix} \begin{bmatrix} b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 \\ d_1 & d_2 & d_3 & d_4 \end{bmatrix} |\Omega^e| \tag{33}$$

$$\Omega^e = \frac{1}{6} \begin{vmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{vmatrix} \tag{34}$$

$$P^e = \int_{\Omega^e} \sigma^e \xi_i^e \xi_j^e \, d\Omega^e \qquad i,j = 1,\ldots,4 \tag{35}$$

$$P^e = \sigma^e \frac{|\Omega^e|}{20} \begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix} \tag{36}$$

$$\boldsymbol{f}^e = \boldsymbol{f}_g^e + \boldsymbol{f}_s^e + \boldsymbol{f}_n^e \tag{37}$$

$$\begin{aligned} \boldsymbol{f}_g^e &= \int_{\Omega^e} \nabla \xi_i^{eT} \left(\frac{K}{\mu}\gamma\right)^e \nabla z \, d\Omega^e \qquad i = 1,\ldots,4 \\ &= \left(\frac{\gamma}{\mu}\right)^e \begin{bmatrix} b_1 & c_1 & d_1 \\ b_2 & c_2 & d_2 \\ b_3 & c_3 & d_3 \\ b_4 & c_4 & d_4 \end{bmatrix} \begin{bmatrix} k_{xz} \\ k_{yz} \\ k_{zz} \end{bmatrix} |\Omega^e| \end{aligned} \tag{38}$$

$$\begin{aligned} \boldsymbol{f}_s^e &= \int_{\Omega^e} q^e \xi_i^e \, d\Omega^e \qquad i = 1,\ldots,4 \\ &= q^e \frac{|\Omega^e|}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^T \end{aligned} \tag{39}$$

$$\begin{aligned} \boldsymbol{f}_n^e &= -\int_{\Gamma_q^e} q_n^e \xi_i^e \, d\Gamma^e \qquad i = 1,\ldots,3 \\ &= -q_n^e \frac{|\Delta^e|}{3} \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T \end{aligned} \tag{40}$$

3.3.2 Hexahedra

$$\begin{aligned} H^e &= \int_{\Omega^e} \nabla \xi_i^{eT} \left(\frac{K}{\mu}\right)^e \nabla \xi_j^e \, d\Omega^e \\ &= \int_{\Omega^{\hat{e}}} \nabla \hat{\xi}_i^{\,T} \left(\frac{K}{\mu}\right)^e \nabla \hat{\xi}_j \det\left(J_\Psi\right) d\Omega^{\hat{e}} \\ &= \sum_{\ell=1}^{nG} \nabla \hat{\xi}_i \left(\boldsymbol{x}_\ell\right)^T \left(\frac{K}{\mu}\right)^e \nabla \hat{\xi}_j \left(\boldsymbol{x}_\ell\right) \det\left(J_\Psi\right)_\ell w_\ell \qquad i,j = 1,\ldots,8 \end{aligned} \tag{41}$$

$$H^e = \frac{1}{\mu^e} \sum_{\ell=1}^{nG} \begin{bmatrix} b_1 & c_1 & d_1 \\ b_2 & c_2 & d_2 \\ \vdots & \vdots & \vdots \\ b_8 & c_8 & d_8 \end{bmatrix}_\ell \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix} \begin{bmatrix} b_1 & b_2 & \cdots & b_8 \\ c_1 & c_2 & \cdots & c_8 \\ d_1 & d_2 & \cdots & d_8 \end{bmatrix}_\ell \det\left(J_\Psi\right)_\ell w_\ell \tag{42}$$

$$\begin{aligned} P^e &= \int_{\Omega^e} \sigma^e \xi_i^e \xi_j^e \, d\Omega^e \\ &= \int_{\Omega^{\hat{e}}} \sigma^e \hat{\xi}_i \hat{\xi}_j \det\left(J_\Psi\right) \, d\Omega^{\hat{e}} \\ &= \sigma^e \sum_{\ell=1}^{nG} \hat{\xi}_i \left(\boldsymbol{x}_\ell\right) \hat{\xi}_j \left(\boldsymbol{x}_\ell\right) \det\left(J_\Psi\right)_\ell w_\ell \qquad i,j = 1,\ldots,8 \end{aligned} \tag{43}$$

$$\begin{aligned} P^e =& \sigma^e \begin{bmatrix} \hat{\xi}_1^1 & \hat{\xi}_1^2 & \cdots & \hat{\xi}_1^{nG} \\ \hat{\xi}_2^1 & \hat{\xi}_2^2 & \cdots & \hat{\xi}_2^{nG} \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\xi}_8^1 & \hat{\xi}_8^2 & \cdots & \hat{\xi}_8^{nG} \end{bmatrix} \begin{bmatrix} \det\left(J_\Psi\right)_1 w_1 & & \\ & \ddots & \\ & & \det\left(J_\Psi\right)_{nG} w_{nG} \end{bmatrix} \\ & \begin{bmatrix} \hat{\xi}_1^1 & \hat{\xi}_2^1 & \cdots & \hat{\xi}_8^1 \\ \hat{\xi}_1^2 & \hat{\xi}_2^2 & \cdots & \hat{\xi}_8^2 \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\xi}_1^{nG} & \hat{\xi}_2^{nG} & \cdots & \hat{\xi}_8^{nG} \end{bmatrix} \end{aligned} \tag{44}$$

$$\boldsymbol{f}^e = \boldsymbol{f}_g^e + \boldsymbol{f}_s^e + \boldsymbol{f}_n^e \tag{45}$$

$$
\begin{aligned}
\boldsymbol{f}_g^e &= \int_{\Omega^e} \nabla \xi_i^{eT} \left(\frac{K}{\mu}\gamma\right)^e \nabla z \, d\Omega^e \\
&= \int_{\Omega^{\hat{e}}} \nabla \hat{\xi}_i^{\,T} \left(\frac{K}{\mu}\gamma\right)^e \nabla \hat{z} \det\left(J_\Psi\right) \, d\Omega^{\hat{e}} \\
&= \sum_{\ell=1}^{nG} \nabla \hat{\xi}_i \left(\boldsymbol{x}_\ell\right)^T \left(\frac{K}{\mu}\gamma\right)^e \nabla \hat{z} \det\left(J_\Psi\right)_\ell w_\ell \qquad i = 1, \ldots, 8 \\
&= \left(\frac{\gamma}{\mu}\right)^e \begin{bmatrix} b_1 & c_1 & d_1 \\ b_2 & c_2 & d_2 \\ \vdots & \vdots & \vdots \\ b_8 & c_8 & d_8 \end{bmatrix}_\ell \begin{bmatrix} k_{xz} \\ k_{yz} \\ k_{zz} \end{bmatrix} \det\left(J_\Psi\right)_\ell w_\ell
\end{aligned} \tag{46}
$$

$$
\begin{aligned}
\boldsymbol{f}_s^e &= \int_{\Omega^e} q^e \xi_i^e \, d\Omega^e \qquad i = 1, \ldots, 8 \\
&= ??
\end{aligned} \tag{47}
$$

$$
\begin{aligned}
\boldsymbol{f}_n^e &= -\int_{\Gamma_q^e} q_n^e \xi_i^e \, d\Gamma^e \qquad i = 1, \ldots, 4 \\
&= ??
\end{aligned} \tag{48}
$$