GRES: Report

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1 Mathematical models

Mass conservation equation:

1.1 Single-phase slightly compressible flow in porous media

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

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 fluid flow injected or produced per unit volume [1/T].

The physical quantities in the dimensional analysis of each parameter are as follows: $L \rightarrow$ length, $P \rightarrow$ pressure, $T \rightarrow$ time.

$\boldsymbol{v}$ 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.

1.2 Variably saturated slightly compressible flow in porous media

$$\sigma(S_w)\frac{\partial p}{\partial t} + \nabla \cdot \boldsymbol{v} = q \tag{4}$$

where S_w is the water saturation ($0 \leq S_w \leq 1$) and the storage coefficient, which depends on S_w, is expressed as:

$$\sigma = S_w(\alpha + \beta\phi) + \phi\frac{dS_w}{dp} \tag{5}$$

Darcy's velocity modified to account for the simultaneous presence of air and water in the pore space:

$$\boldsymbol{v} = -\lambda K \nabla(p + \gamma z) \tag{6}$$

where $\lambda(S_w) = k_r(S_w)/\mu$ is the so-called *mobility factor* and $k_r(S_w)$ is the relative permeability. Substituting Eq. (6) into (4) gives the classical pressure form of the Richards' equation:

$$\nabla \cdot [\lambda K \nabla (p + \gamma z)] = \sigma(S_w)\frac{\partial p}{\partial t} - q \tag{7}$$

Let S_w^* denote the effective water saturation:

$$S_w^* = \frac{S_w - S_{wr}}{1 - S_{wr}} \tag{8}$$

where S_{wr} is the residual saturation of water. Capillary curves relate pressure and effective saturation, usually in a nonlinear form, that can be expressed as:

$$S_w^* = S_w^*(p) \tag{9}$$

Much in a similar way, another nonlinear relationship gives the relative permeability in terms of pressure:

$$k_r = k_r(p) \tag{10}$$

In the Matlab code, the two relationships (9) and (10) are provided in a tabular format.

2 Numerical models

2.1 Single-phase slightly compressible flow in porous media

2.1.1 FEM

Let $\mathcal{N}$ be the set of nodes in the discretized domain.

$$p \approx \hat{p}(\boldsymbol{x}, t) = \sum_{i \in \mathcal{N}} p_i(t)\xi_i(\boldsymbol{x}) \tag{11}$$

$$L(\hat{p}) = \nabla \cdot \left[\frac{K}{\mu} \nabla \left(\hat{p} + \gamma z \right) \right] - \sigma \frac{\partial \hat{p}}{\partial t} + q \tag{12}$$

$$\int_\Omega L(\hat{p}) \xi_i \, d\Omega = 0 \qquad i \in \mathcal{N} \tag{13}$$

$$- \int_\Omega \nabla \xi_i{}^T \left[\frac{K}{\mu} \nabla \left(\hat{p} + \gamma z \right) \right] d\Omega + \int_\Gamma \left[\frac{K}{\mu} \nabla (\hat{p} + \gamma z) \cdot \boldsymbol{n} \right] \xi_i \, d\Gamma \\ - \int_\Omega \sigma \frac{\partial \hat{p}}{\partial t} \xi_i \, d\Omega + \int_\Omega q \xi_i \, d\Omega = 0 \qquad i \in \mathcal{N} \tag{14}$$

$$\frac{K}{\mu} \nabla (p + \gamma z) \cdot \boldsymbol{n} = q_n \tag{15}$$

$$\int_\Omega \nabla \xi_i{}^T \frac{K}{\mu} \nabla \hat{p} \, d\Omega + \int_\Omega \sigma \frac{\partial \hat{p}}{\partial t} \xi_i \, d\Omega + \int_\Omega \nabla \xi_i{}^T \frac{K}{\mu} \gamma \nabla z \, d\Omega \\ - \int_\Omega q \xi_i \, d\Omega - \int_{\Gamma_q} q_n \xi_i \, d\Gamma = 0 \qquad i \in \mathcal{N} \tag{16}$$

$$\int_\Omega \left(\sum_{j \in \mathcal{N}} \nabla \xi_i{}^T \frac{K}{\mu} \nabla \xi_j p_j \right) d\Omega + \int_\Omega \left(\sum_{j \in \mathcal{N}} \sigma \xi_i \xi_j \frac{\partial p_j}{\partial t} \right) d\Omega \\ + \int_\Omega \nabla \xi_i{}^T \frac{K}{\mu} \gamma \nabla z \, d\Omega - \int_\Omega q \xi_i \, d\Omega - \int_{\Gamma_q} q_n \xi_i \, d\Gamma = 0 \qquad i \in \mathcal{N} \tag{17}$$

$$H \boldsymbol{p} + P \frac{\partial \boldsymbol{p}}{\partial t} + \boldsymbol{f} = 0 \tag{18}$$

where $\boldsymbol{p} = [p_1, p_2, \ldots, p_l]^T$. Let $\mathcal{E}$ be the set of cells in the discretized domain.

$$H_{ij} = \sum_{e \in \mathcal{E}} H_{ij}^e = \sum_{e \in \mathcal{E}} \frac{1}{\mu} \int_{\Omega^e} \nabla \xi_i^{eT} K^e \nabla \xi_j^e \, d\Omega \tag{19}$$

$$P_{ij} = \sum_{e \in \mathcal{E}} P_{ij}^e = \sum_{e \in \mathcal{E}} \int_{\Omega^e} \sigma^e \xi_i^e \xi_j^e \, d\Omega \tag{20}$$

$$f_i = \sum_{e \in \mathcal{E}} f_i^e = \sum_{e \in \mathcal{E}} \left[\frac{\gamma}{\mu} \int_{\Omega^e} \nabla \xi_i^{eT} K^e \nabla z \, d\Omega - \int_{\Omega^e} q^e \xi_i^e \, d\Omega - \int_{\Gamma_q^e} q_n^e \xi_i^e \, d\Gamma \right] \tag{21}$$

2.1.2 FV-TPFA

$$p \approx \hat{p}(\boldsymbol{x}, t) = \sum_{e \in \mathcal{E}} p_e(t) \xi_e(\boldsymbol{x}) \tag{22}$$

where

$$\xi_e(\boldsymbol{x}) = \begin{cases} 1 & \boldsymbol{x} \in e \\ 0 & \boldsymbol{x} \notin e \end{cases} \tag{23}$$

The integration on Ω reduces to Ω^e

$$\int_{\Omega^e} \sigma \frac{\partial \hat{p}}{\partial t} \, d\Omega + \int_{\Omega^e} \nabla \cdot \boldsymbol{v} \, d\Omega - \int_{\Omega^e} q \, d\Omega = 0 \qquad e \in \mathcal{E} \tag{24}$$

Divergence theorem

$$\int_{\Omega^e} \sigma \frac{\partial \hat{p}}{\partial t} \, d\Omega + \oint_{\partial e} \boldsymbol{v} \cdot \boldsymbol{n} \, d\Gamma - \int_{\Omega^e} q \, d\Omega = 0 \qquad e \in \mathcal{E} \tag{25}$$

Assuming that $\mathcal{F}^e \subset \mathcal{F}$ is the set of faces of e

$$\oint_{\partial e} \boldsymbol{v} \cdot \boldsymbol{n} \, d\Gamma = \sum_{f \in \mathcal{F}^e} q_{ef} \tag{26}$$

Using the midpoint rule we can express the flux across face f ($\boldsymbol{c}_f$ face midpoint) as

$$q_{ef} = \int_{\Delta^f} \boldsymbol{v} \cdot \boldsymbol{n} \, d\Delta \approx -\Delta^f \frac{K_e}{\mu_e} \left[\nabla \left(\hat{p} + \gamma z \right) \right] (\boldsymbol{c}_f) \cdot \boldsymbol{n}_f \tag{27}$$

We can approximate the potential gradient as follows:

$$q_{ef} \approx \Delta^f \frac{K_e}{\mu_e} \frac{\boldsymbol{l}_{ef}}{\|\boldsymbol{l}_{ef}\|_2^2} \cdot \boldsymbol{n}_f \left[p_e - \pi_f + \gamma (z_e - z_f) \right] = T_{ef} \left[p_e - \pi_f + \gamma (z_e - z_f) \right] \tag{28}$$

with

$$T_{ef} = \Delta^f \frac{K_e}{\mu_e} \frac{\boldsymbol{l}_{ef}}{\|\boldsymbol{l}_{ef}\|_2^2} \cdot \boldsymbol{n}_f \tag{29}$$

<u>half-face transmissibility</u>, i.e., transmissibility of face f on the side of element e. If e' is the neighboring element of e sharing face f, for continuity reasons

$$q_{ef} = q_{e'f} \quad \rightarrow \quad T_{ef} \left[p_e - \pi_f + \gamma (z_e - z_f) \right] = T_{e'f} \left[p_{e'} - \pi_f + \gamma (z_{e'} - z_f) \right] \tag{30}$$

$$q_{ee'} = T_f \left[p_e - p_{e'} + \gamma (z_e - z_{e'}) \right] \tag{31}$$

$$T_f = \left(T_{ef}^{-1} + T_{e'f}^{-1} \right)^{-1} \tag{32}$$

We will use $q_{ee'}$ in eq. 21 for internal faces and q_{ef} for external faces with prescribed pressure or flux. In the first case π_f is given, in the latter q_{ef} itself is given. By splitting the pressure and gravity contributions and solving the integrals for the accumulation and source terms we obtain:

$$\sigma_e |\Omega^e| \frac{\partial \hat{p}}{\partial t} + \sum_{e' \in \mathcal{C}^e} q_{ee'}^p + \sum_{f \in \mathcal{F}_\Gamma^e} q_{ef}^p - q|\Omega^e| + \sum_{e' \in \mathcal{C}^e} q_{ee'}^z + \sum_{f \in \mathcal{F}_\Gamma^e} q_{ef}^z = 0 \qquad e \in \mathcal{E} \tag{33}$$

$$q_{ee'}^p = T_f (p_e - p_{e'}) \qquad\qquad q_{ee'}^z = T_f \gamma (z_e - z_{e'}) \tag{34}$$

$$q_{ef}^p = T_{ef} (p_e - \pi_f) \qquad\qquad q_{ef}^z = T_{ef} \gamma (z_e - z_f) \tag{35}$$

$\mathcal{C}^e$ is the set of neighboring element of e.

$$H \boldsymbol{p} + P \frac{\partial \boldsymbol{p}}{\partial t} + \boldsymbol{f} = 0 \tag{36}$$

2.2 Variably saturated slightly compressible flow in porous media

Richards' equation discretized in space, following the same approach as in the single-phase flow problem reads:

$$\sigma_e|\Omega^e|\frac{\partial \hat{p}}{\partial t}+\sum_{e'\in\mathcal{C}^e} q^p_{ee'}+\sum_{f\in\mathcal{F}^e_\Gamma} q^p_{ef}-q|\Omega^e|+\sum_{e'\in\mathcal{C}^e} q^z_{ee'}+\sum_{f\in\mathcal{F}^e_\Gamma} q^z_{ef}=0 \qquad e\in\mathcal{E} \quad (37)$$

where:

$$\sigma_e = S^e_w(\alpha+\beta\phi)+\phi\frac{dS^e_w}{dp} \quad (38)$$

$$q^p_{ee'} = \lambda_u T_f(p_e-p_{e'}) \qquad q^z_{ee'} = \lambda_u T_f\gamma(z_e-z_{e'}) \quad (39)$$

$$q^p_{ef} = \lambda_u T_{ef}(p_e-\pi_f) \qquad q^z_{ef} = \lambda_u T_{ef}\gamma(z_e-z_f) \quad (40)$$

$\lambda_u = k_r(S^u_w)/\mu$ is the mobility factor evaluated at the *upstream element*. Let Ψ be the pressure potential:

$$\Psi = p_e - p_{e'} + \gamma(z_e-z_{e'}) \quad (41)$$

then

$$S^u_w = \begin{cases} S^e_w & \text{if } \Psi \geq 0 \\ S^{e'}_w & \text{if } \Psi < 0 \end{cases} \quad (42)$$

$$H\boldsymbol{p}+P\frac{\partial \boldsymbol{p}}{\partial t}+\boldsymbol{f}=0 \quad (43)$$

The system above is nonlinear, so it requires a nonlinear solver (Picard or Newton) to be solved.

2.3 Time integration

$$0\leq\theta\leq 1 \quad (44)$$

$$\tau = t+\theta\Delta t \quad (45)$$

$$\boldsymbol{p}_\tau = \theta\boldsymbol{p}_{t+\Delta t}+(1-\theta)\boldsymbol{p}_t \quad (46)$$

$$\boldsymbol{f}_\tau = \theta\boldsymbol{f}_{t+\Delta t}+(1-\theta)\boldsymbol{f}_t \quad (47)$$

$$\left.\frac{\partial \boldsymbol{p}}{\partial t}\right|_\tau = \frac{\boldsymbol{p}_{t+\Delta t}-\boldsymbol{p}_t}{\Delta t} \quad (48)$$

$$\boldsymbol{R}(\boldsymbol{p}_{t+\Delta t})=\boldsymbol{0} \quad \rightarrow$$

$$\left(\theta H_\tau+\frac{P_\tau}{\Delta t}\right)\boldsymbol{p}_{t+\Delta t} = \left[\frac{P_\tau}{\Delta t}-(1-\theta)H_\tau\right]\boldsymbol{p}_t-\boldsymbol{f}_\tau \quad (49)$$

This is the set of equations originating from the spatial/temporal discretization of the problem PDEs, written for each cell/node of the domain. Such a system of equations is linear or nonlinear, depending on the type of the problem. In case of nonlinear problems, an adequate solver needs to be provided. Usually, this is an iterative Newton-like scheme:

$$J^{(m)}\delta\boldsymbol{p} = -\boldsymbol{R}(\boldsymbol{p}^{(m)}_{t+\Delta t}) \tag{50}$$

with

$$\boldsymbol{p}^{(m+1)}_{t+\Delta t} = \boldsymbol{p}^{(m)}_{t+\Delta t} + \delta\boldsymbol{p} \tag{51}$$

and the Jacobian matrix

$$J^{(m)} = \frac{\partial \boldsymbol{R}(\boldsymbol{p}^{(m)}_{t+\Delta t})}{\partial \boldsymbol{p}_{t+\Delta t}} \tag{52}$$

An exact Newton scheme is obtained whenever the derivatives in (52) are computed exactly. In the Picard method, some terms of the exact Jacobian are dropped.

3 FE Matrices

3.1 Tetrahedra

$$\xi^e_i(x,y,z) = a_i + b_i x + c_i y + d_i z \qquad i = 1,\dots,4 \tag{53}$$

where

$$\begin{bmatrix} a_1 & a_2 & a_3 & a_4 \\ b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 \\ d_1 & d_2 & d_3 & d_4 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{bmatrix}^{-1} \tag{54}$$

The volume of any tetrahedron is given by:

$$\Omega^e = \frac{1}{6}\begin{vmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{vmatrix} \tag{55}$$

3.2 Hexahedra

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

$$\begin{aligned} \Psi : \mathbb{R}^3 &\longrightarrow \mathbb{R}^3 \\ \hat{\boldsymbol{x}} \in \hat{e} &\longmapsto \boldsymbol{x} = \Psi(\hat{\boldsymbol{x}}) \in e. \end{aligned} \tag{56}$$

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

$$\xi_i(\hat{x},\hat{y},\hat{z}) = \frac{1}{8}(1+\hat{x}\hat{x}_i)(1+\hat{y}\hat{y}_i)(1+\hat{z}\hat{z}_i) \qquad i = 1,\dots,8 \tag{57}$$

where ξ_i is the basis function of the i-th node and $\hat{x}_i$, $\hat{y}_i$, $\hat{z}_i$ are its coordinates, implying that $\hat{x}_i, \hat{y}_i, \hat{z}_i = \pm 1$ for $i = 1, \dots, 8$. Using eqs. (57), Ψ is simply given by:

$$\boldsymbol{x} = \Psi\left(\hat{\boldsymbol{x}}\right) = \begin{bmatrix} x_1 & x_2 & \dots & x_8 \\ y_1 & y_2 & \dots & y_8 \\ z_1 & z_2 & \dots & z_8 \end{bmatrix} \begin{bmatrix} \xi_1\left(\hat{\boldsymbol{x}}\right) \\ \xi_2\left(\hat{\boldsymbol{x}}\right) \\ \vdots \\ \xi_8\left(\hat{\boldsymbol{x}}\right) \end{bmatrix} = X\boldsymbol{\xi}\left(\hat{\boldsymbol{x}}\right). \tag{58}$$

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:

$$\begin{bmatrix} \frac{\partial \xi_i}{\partial x} \\ \frac{\partial \xi_i}{\partial y} \\ \frac{\partial \xi_i}{\partial z} \end{bmatrix} = J_\Psi^{-1} \begin{bmatrix} \frac{\partial \xi_i}{\partial \hat{x}} \\ \frac{\partial \xi_i}{\partial \hat{y}} \\ \frac{\partial \xi_i}{\partial \hat{z}} \end{bmatrix} \tag{59}$$

Here, J_Ψ is the Jacobian of the isoparametric transformation:

$$J_\Psi = \begin{bmatrix} \frac{\partial \xi_1(\hat{\boldsymbol{x}})}{\partial \hat{x}} & \frac{\partial \xi_2(\hat{\boldsymbol{x}})}{\partial \hat{x}} & \dots & \frac{\partial \xi_8(\hat{\boldsymbol{x}})}{\partial \hat{x}} \\ \frac{\partial \xi_1(\hat{\boldsymbol{x}})}{\partial \hat{y}} & \frac{\partial \xi_2(\hat{\boldsymbol{x}})}{\partial \hat{y}} & \dots & \frac{\partial \xi_8(\hat{\boldsymbol{x}})}{\partial \hat{y}} \\ \frac{\partial \xi_1(\hat{\boldsymbol{x}})}{\partial \hat{z}} & \frac{\partial \xi_2(\hat{\boldsymbol{x}})}{\partial \hat{z}} & \dots & \frac{\partial \xi_8(\hat{\boldsymbol{x}})}{\partial \hat{z}} \end{bmatrix} \begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ \vdots & \vdots & \vdots \\ x_8 & y_8 & z_8 \end{bmatrix} = J_\xi\left(\hat{\boldsymbol{x}}\right) X \tag{60}$$

Integrals in eqs. (19), (20) and (21) 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 thus 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 expressed in eq. (59) are simply given by:

$$\begin{bmatrix} b_1 & b_2 & \cdots & b_8 \\ c_1 & c_2 & \cdots & c_8 \\ d_1 & d_2 & \cdots & d_8 \end{bmatrix}_\ell = \begin{bmatrix} j_{11}^{-1} & j_{12}^{-1} & j_{13}^{-1} \\ j_{21}^{-1} & j_{22}^{-1} & j_{23}^{-1} \\ j_{31}^{-1} & j_{32}^{-1} & j_{33}^{-1} \end{bmatrix}_\ell \begin{bmatrix} \frac{\partial \xi_1}{\partial \hat{x}} & \frac{\partial \xi_2}{\partial \hat{x}} & \cdots & \frac{\partial \xi_8}{\partial \hat{x}} \\ \frac{\partial \xi_1}{\partial \hat{y}} & \frac{\partial \xi_2}{\partial \hat{y}} & \cdots & \frac{\partial \xi_8}{\partial \hat{y}} \\ \frac{\partial \xi_1}{\partial \hat{z}} & \frac{\partial \xi_2}{\partial \hat{z}} & \cdots & \frac{\partial \xi_8}{\partial \hat{z}} \end{bmatrix}_\ell \tag{61}$$

3.3 Flow

3.3.1 Tetrahedra

$$H^e = \frac{1}{\mu} \int_{\Omega^e} \nabla \xi_i^{e\,T} K^e \nabla \xi_j^e \, d\Omega, \qquad i, j = 1, \dots, 4 \tag{62}$$

$$H^e = \frac{1}{\mu} \begin{bmatrix} b_1 & c_1 & d_1 \\ b_2 & c_2 & d_2 \\ b_3 & c_3 & d_3 \\ b_4 & c_4 & d_4 \end{bmatrix} \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix}^e \begin{bmatrix} b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 \\ d_1 & d_2 & d_3 & d_4 \end{bmatrix} |\Omega^e| \tag{63}$$

$$P^e = \int_{\Omega^e} \sigma^e \xi_i^e \xi_j^e \, d\Omega \qquad i,j = 1,\dots,4 \tag{64}$$

$$P^e = \sigma^e \frac{|\Omega^e|}{20} \begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix} \tag{65}$$

$$\boldsymbol{f}^e = \boldsymbol{f}_g^e + \boldsymbol{f}_s^e + \boldsymbol{f}_n^e \tag{66}$$

$$\begin{aligned} \boldsymbol{f}_g^e &= \frac{\gamma}{\mu} \int_{\Omega^e} \nabla \xi_i^{eT} K^e \nabla z \, d\Omega \qquad i = 1,\dots,4 \\ &= \frac{\gamma}{\mu} \begin{bmatrix} b_1 & c_1 & d_1 \\ b_2 & c_2 & d_2 \\ b_3 & c_3 & d_3 \\ b_4 & c_4 & d_4 \end{bmatrix} \begin{bmatrix} k_{xz} \\ k_{yz} \\ k_{zz} \end{bmatrix} |\Omega^e| \end{aligned} \tag{67}$$

$$\begin{aligned} \boldsymbol{f}_s^e &= \int_{\Omega^e} q^e \xi_i^e \, d\Omega \qquad i = 1,\dots,4 \\ &= q^e \frac{|\Omega^e|}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^T \end{aligned} \tag{68}$$

$$\begin{aligned} \boldsymbol{f}_n^e &= -\int_{\Gamma_q^e} q_n^e \xi_i^e \, d\Gamma \qquad i = 1,\dots,3 \\ &= -q_n^e \frac{|\Delta^e|}{3} \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T \end{aligned} \tag{69}$$

3.3.2 Hexahedra

We indicate by ξ_i (without the superscript e) the basis function of the i-th node of the reference element and by $\hat{\Omega}$ its volume.

$$\begin{aligned} H^e &= \frac{1}{\mu} \int_{\Omega^e} \nabla \xi_i^{eT} K^e \nabla \xi_j^e \, d\Omega \\ &= \frac{1}{\mu} \int_{\hat{\Omega}} \nabla \xi_i^T K^e \nabla \xi_j \det(J_\Psi^e) \, d\Omega \\ &= \frac{1}{\mu} \sum_{\ell=1}^{nG} \nabla \xi_i (\boldsymbol{x}_\ell)^T K^e \nabla \xi_j (\boldsymbol{x}_\ell) \det(J_\Psi^e)_\ell \, w_\ell \qquad i,j = 1,\dots,8 \end{aligned} \tag{70}$$

$$H^e = \frac{1}{\mu} \sum_{\ell=1}^{nG} \begin{bmatrix} b_1 & c_1 & d_1 \\ b_2 & c_2 & d_2 \\ \vdots & \vdots & \vdots \\ b_8 & c_8 & d_8 \end{bmatrix}_\ell \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix}^e \begin{bmatrix} b_1 & b_2 & \cdots & b_8 \\ c_1 & c_2 & \cdots & c_8 \\ d_1 & d_2 & \cdots & d_8 \end{bmatrix}_\ell \det(J_\Psi^e)_\ell \, w_\ell \tag{71}$$

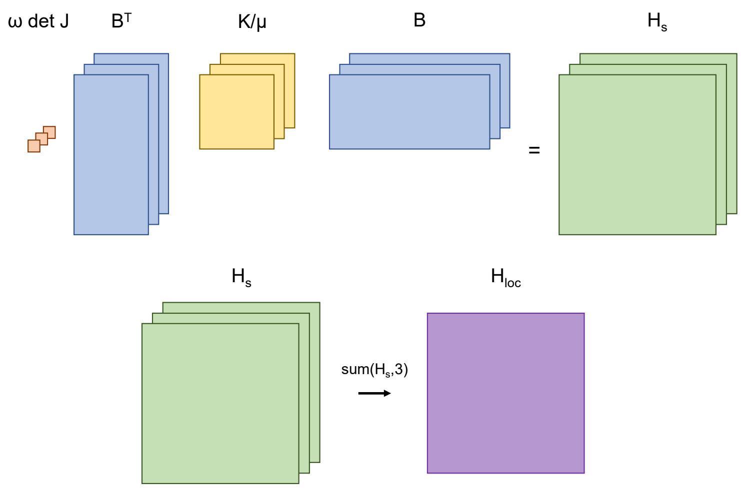

Figure 1: Schematic representation of the way in which the local stiffness matrices are computed in the Matlab code.

$$\begin{aligned} P^e &= \int_{\Omega^e} \sigma^e \xi_i^e \xi_j^e \, d\Omega \\ &= \int_{\hat{\Omega}} \sigma^e \xi_i \xi_j \det\left(J_\Psi^e\right) d\Omega \\ &= \sigma^e \sum_{\ell=1}^{nG} \xi_i\left(\boldsymbol{x}_\ell\right) \xi_j\left(\boldsymbol{x}_\ell\right) \det\left(J_\Psi^e\right)_\ell w_\ell \qquad i,j = 1,\ldots,8 \end{aligned} \tag{72}$$

$$\begin{aligned} P^e =& \sigma^e \begin{bmatrix} \xi_1^1 & \xi_1^2 & \cdots & \xi_1^{nG} \\ \xi_2^1 & \xi_2^2 & \cdots & \xi_2^{nG} \\ \vdots & \vdots & \ddots & \vdots \\ \xi_8^1 & \xi_8^2 & \cdots & \xi_8^{nG} \end{bmatrix} \begin{bmatrix} \det\left(J_\Psi^e\right)_1 w_1 & & \\ & \ddots & \\ & & \det\left(J_\Psi^e\right)_{nG} w_{nG} \end{bmatrix} \\ & \begin{bmatrix} \xi_1^1 & \xi_2^1 & \cdots & \xi_8^1 \\ \xi_1^2 & \xi_2^2 & \cdots & \xi_8^2 \\ \vdots & \vdots & \ddots & \vdots \\ \xi_1^{nG} & \xi_2^{nG} & \cdots & \xi_8^{nG} \end{bmatrix} \end{aligned} \tag{73}$$

where ξ_i^ℓ is the basis function of node i evaluated at the ℓ-th Gauss point.

$$\boldsymbol{f}^e = \boldsymbol{f}_g^e + \boldsymbol{f}_s^e + \boldsymbol{f}_n^e \tag{74}$$

$$
\begin{aligned}
\boldsymbol{f}_g^e &= \frac{\gamma}{\mu}\int_{\Omega^e} \nabla\xi_i^{eT} K^e \nabla z \, d\Omega \\
&= \frac{\gamma}{\mu}\int_{\hat{\Omega}} \nabla\xi_i^T K^e \nabla\hat{z} \det\left(J_\Psi^e\right)\, d\Omega \\
&= \frac{\gamma}{\mu}\sum_{\ell=1}^{nG} \nabla\xi_i\left(\boldsymbol{x}_\ell\right)^T K^e \nabla\hat{z} \det\left(J_\Psi^e\right)_\ell w_\ell \qquad i = 1,\dots,8 \\
&= \frac{\gamma}{\mu}\sum_{\ell=1}^{nG} \begin{bmatrix} b_1 & c_1 & d_1 \\ b_2 & c_2 & d_2 \\ \vdots & \vdots & \vdots \\ b_8 & c_8 & d_8 \end{bmatrix}_\ell \begin{bmatrix} k_{xz} \\ k_{yz} \\ k_{zz} \end{bmatrix}^e \det\left(J_\Psi^e\right)_\ell w_\ell
\end{aligned} \tag{75}
$$

$$
\begin{aligned}
\boldsymbol{f}_s^e &= \int_{\Omega^e} q^e \xi_i^e \, d\Omega \\
&= \int_{\hat{\Omega}} q^e \xi_i \det\left(J_\Psi^e\right) d\Omega \qquad i = 1,\dots,8 \\
&= q^e \begin{bmatrix} \xi_1^1 & \xi_1^2 & \cdots & \xi_1^{nG} \\ \xi_2^1 & \xi_2^2 & \cdots & \xi_2^{nG} \\ \vdots & \vdots & \ddots & \vdots \\ \xi_8^1 & \xi_8^2 & \cdots & \xi_8^{nG} \end{bmatrix} \begin{bmatrix} \det\left(J_\Psi^e\right)_1 w_1 \\ \det\left(J_\Psi^e\right)_2 w_2 \\ \cdots \\ \det\left(J_\Psi^e\right)_{nG} w_{nG} \end{bmatrix}
\end{aligned} \tag{76}
$$

$$
\begin{aligned}
\boldsymbol{f}_n^e &= -\int_{\Gamma_q^e} q_n^e \xi_i^e \, d\Gamma^e \qquad i = 1,\dots,4 \\
&= -q_n^e \frac{|\Delta^e|}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^T
\end{aligned} \tag{77}
$$

4 FV matrices

4.1 Single-phase slightly compressible flow in porous media

$$
H_{e,:} = \begin{cases} H_{ee} = \sum_{f \in \mathcal{F}^e \cap \mathcal{F}^{e'}} T_f \\ H_{ee'} = -T_f \end{cases} \qquad \forall e' \in \mathcal{C}^e \qquad \forall e \in \mathcal{E} \tag{78}
$$

H is characterized by a seven-point stencil, which is typical of FV-TPFA discretizations on hexahedral meshes. There is also an additional contribution to the diagonal entry when the element lies on the Dirichlet boundary:

$$
H_{ee} = T_{ef} \qquad \text{with } f \in \mathcal{F}_{\Gamma_p}^e \tag{79}
$$

The capacity matrix is diagonal with entries:

$$
P_{ee} = \sigma^e |\Omega^e| \qquad \forall e \in \mathcal{E} \tag{80}
$$

$$
\boldsymbol{f}_e = \boldsymbol{f}_e^g + \boldsymbol{f}_e^s + \boldsymbol{f}_e^n \tag{81}
$$

$$\boldsymbol{f}_e^g = \sum_{e' \in \mathcal{C}^e} \gamma T_f (z_e - z_{e'}) \qquad \text{with } f \in \mathcal{F}^e \cap \mathcal{F}^{e'} \tag{82}$$

$$\boldsymbol{f}_e^s = q^e |\Omega^e| \tag{83}$$

$$\boldsymbol{f}_e^n = q_f^e |\Delta^e| \qquad \forall f \in \mathcal{F}^e_{\Gamma_q} \tag{84}$$

4.2 Variably saturated slightly compressible flow in porous media

$$H_{e,:} = \begin{cases} H_{ee} = \sum_{f \in \mathcal{F}^e \cap \mathcal{F}^{e'}} \lambda_f T_f \\ H_{ee'} = -\lambda_f T_f \end{cases} \qquad \forall e' \in \mathcal{C}^e \qquad \forall e \in \mathcal{E} \tag{85}$$

$$P_{ee} = \sigma^e (S_w^e) |\Omega^e| \qquad \forall e \in \mathcal{E} \tag{86}$$

$$\boldsymbol{f}_e = \boldsymbol{f}_e^g + \boldsymbol{f}_e^s + \boldsymbol{f}_e^n \tag{87}$$

$$\boldsymbol{f}_e^g = \sum_{e' \in \mathcal{C}^e} \gamma \lambda_f T_f (z_e - z_{e'}) \qquad \text{with } f \in \mathcal{F}^e \cap \mathcal{F}^{e'} \tag{88}$$

$$\boldsymbol{f}_e^s = q^e |\Omega^e| \tag{89}$$

$$\boldsymbol{f}_e^n = q_f^e |\Delta^e| \qquad \forall f \in \mathcal{F}^e_{\Gamma_q} \tag{90}$$

Jacobian matrix

Picard

$$J^{(m)} = \theta H_\tau^{(m)} + \frac{P_\tau^{(m)}}{\Delta t} \tag{91}$$

Newton

$$J^{(m)} = \theta H_\tau^{(m)} + \frac{P_\tau^{(m)}}{\Delta t} + J1^{(m)} + J2^{(m)} \tag{92}$$

$J1^{(m)}$ and $J2^{(m)}$ gather the derivatives of the nonlinear terms:

$$\begin{aligned} J1^{(m)} &= \theta \frac{\partial H_\tau^{(m)}}{\partial \boldsymbol{p}_{t+\Delta t}} \boldsymbol{p}_{t+\Delta t} + (1-\theta) \frac{\partial H_\tau^{(m)}}{\partial \boldsymbol{p}_{t+\Delta t}} \boldsymbol{p}_t + \frac{\boldsymbol{f}_\tau^{(m)}}{\partial \boldsymbol{p}_{t+\Delta t}} \\ &= \frac{\partial H_\tau^{(m)}}{\partial \boldsymbol{p}_{t+\Delta t}} \boldsymbol{p}_\tau + \frac{\boldsymbol{f}_\tau^{(m)}}{\partial \boldsymbol{p}_{t+\Delta t}} \\ &= \frac{\partial H_\tau^{(m)}}{\partial \boldsymbol{p}_\tau} \frac{\partial \boldsymbol{p}_\tau}{\partial \boldsymbol{p}_{t+\Delta t}} \boldsymbol{p}_\tau + \frac{\partial \boldsymbol{f}_\tau^{(m)}}{\partial \boldsymbol{p}_\tau} \frac{\partial \boldsymbol{p}_\tau}{\partial \boldsymbol{p}_{t+\Delta t}} \end{aligned} \tag{93}$$

$$\begin{aligned} J2^{(m)} &= \frac{1}{\Delta t} \frac{\partial P_\tau^{(m)}}{\partial \boldsymbol{p}_{t+\Delta t}} \\ &= \frac{1}{\Delta t} \frac{\partial P_\tau^{(m)}}{\partial \boldsymbol{p}_\tau} \frac{\partial \boldsymbol{p}_\tau}{\partial \boldsymbol{p}_{t+\Delta t}} (\boldsymbol{p}_{t+\Delta t} - \boldsymbol{p}_t) \end{aligned} \tag{94}$$

$$J1_{e,u}^{(m)} = \left. \frac{d\lambda}{dp} \right|_\tau^{u,(m)} T_f \left[p_\tau^{e,(m)} - p_\tau^{e',(m)} + \gamma (z_e - z_{e'}) \right] \theta \qquad \forall u \in \mathcal{U}_e \text{ and } \forall e \in \mathcal{E} \tag{95}$$

where $\mathcal{U}_e$ is the set of upstream elements for the shared faces of element e.

$$J2_{e,e}^{(m)} = \frac{1}{\Delta t}\left(\frac{dS_w}{dp}\bigg|_{\tau}^{e,(m)}(\alpha+\beta\phi)+\phi\frac{d^2S_w}{dp^2}\bigg|_{\tau}^{e,(m)}\right)|\Omega^e|\left(p_{t+\Delta t}^{e,(m)}-p_t^e\right)\theta \qquad \forall e\in\mathcal{E} \tag{96}$$

In the Matlab code, the second term with the second derivative of S_w is not computed.