

POREMAPS: A FINITE DIFFERENCE BASED POROUS MEDIA ANISOTROPIC PERMEABILITY SOLVER FOR STOKES FLOW

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A. NOMENCLATURE

The nomenclature table (**Table S1**) covers the essential quantities, indices, and suffix conventions used in this paper. Scalar quantities are given in regular font weight while vectors and tensors are written in boldface.

B. NONDIMENSIONAL BALANCE EQUATIONS

Nondimensional quantities and operators: We introduce the dimensionless length l^* , velocity $\mathbf{v}^*$, and time t^* by the ratio of physical property divided by characteristic property ($\mathcal{L}, \mathcal{V}, \mathcal{T} = \mathcal{L}/\mathcal{V}$) (**Eq. S1**).

$$l^* = \frac{l}{\mathcal{L}} \rightarrow l = l^* \mathcal{L}, \quad \mathbf{v}^* = \frac{\mathbf{v}}{\mathcal{V}} \rightarrow \mathbf{v} = \mathbf{v}^* \mathcal{V} \quad \text{and} \quad t^* = \frac{t}{\mathcal{T}} \rightarrow t = \frac{t^* \mathcal{L}}{\mathcal{V}} \quad (\text{S1})$$

The nondimensional differential operators $\text{grad}(\cdot)$ and $\text{div}(\cdot)$ and time derivative $(\cdot)^*$ are given as follows: (**Eq. S2**):

$$\text{grad}^*(\cdot) = \mathcal{L} \text{grad}(\cdot) \rightarrow \text{grad}(\cdot) = \frac{1}{\mathcal{L}} \text{grad}^*(\cdot) \quad (\text{S2})$$

$$\text{div}^*(\cdot) = \mathcal{L} \text{div}(\cdot) \rightarrow \text{div}(\cdot) = \frac{1}{\mathcal{L}} \text{div}^*(\cdot)$$

$$(\cdot)^* = \mathcal{T} (\cdot)^{\cdot} = \frac{\mathcal{L}}{\mathcal{V}} (\cdot)^{\cdot} \rightarrow (\cdot)^{\cdot} = \frac{\mathcal{V}}{\mathcal{L}} (\cdot)^*$$

This allows for the selection of the pressure and density scale (**Eq. S3**) where ρ_0 is the rest density of the fluid (**Eq. S3**).

$$\rho^* = \frac{\rho}{\rho_0} \rightarrow \rho = \rho_0 \rho^* \quad \text{and} \quad p^* = \frac{p}{\rho_0 \mathcal{V}^2} \rightarrow p = p^* \rho_0 \mathcal{V}^2 \quad (\text{S3})$$

Nondimensional governing equations: For the mutual dependence of pressure p and density ρ we employ the constitutive equation and its derivative (**Eq. S4**):

$$\rho = \rho_0 \left[\frac{p}{K^F} + 1 \right] \rightarrow \dot{\rho} = \rho_0 \frac{\dot{p}}{K^F} \quad (\text{S4})$$



Table S1: Nomenclature

Index and suffix convention		
i, j, k		Indices as subscripts
$(\cdot)$		Time derivative of quantity $(\cdot)$
$*$		Dimensionless quantities and operators
$\tilde{\cdot}$		Quantities displayed in the principal axis system
$\cdot_i, \cdot_{jk}$		Components of vector or coefficient matrix of tensor
Symbol	Unit	Description
$A_i, \bar{A}_i$	[m ²]	Total/effective cross-sectional area
$\partial\mathcal{B}$	[-]	Surface of domain
c	[m s ⁻¹]	Speed of sound
$\mathbf{e}_i$	[-]	Cartesian basis of orthonormal vectors
$\mathbf{h} = -p_{,i}$	[Pa m ⁻¹]	Hydraulic gradient
$\mathbf{I} = \delta_{ij}(\mathbf{e}_i \otimes \mathbf{e}_j) = \mathbf{e}_i \otimes \mathbf{e}_i$	[-]	Second order identity tensor
k_I, k_{II}, k_{III}	[m ²]	Principal permeabilities of $\mathbf{k}$
$\mathbf{k}$	[m ²]	Second order permeability tensor
K^F	[Pa]	Bulk modulus of the fluid
$\mathcal{L}$	[m]	Characteristic length of scale
p	[Pa]	Pressure of the pore fluid
$\mathbf{q}$	[m s ⁻¹]	Darcy velocity
Q	[m ³ s ⁻¹]	Volumetric flow rate
Re	[-]	Reynolds number
$\mathcal{T}$	[s]	Characteristic time scale
$\mathbf{v}$	[m s ⁻¹]	Velocity vector of the fluid
$\mathcal{V}$	[m s ⁻¹]	Characteristic velocity
α	[°]	Presupposed angle
ε	[-]	Convergence criterion
$\mathcal{E}$	[-]	Second order strain tensor
λ_i		Eigenvalues
μ	[Pa s]	Dynamic viscosity of the fluid
ρ_0, ρ	[kg m ⁻³]	Rest density, density of the fluid
σ	[Pa]	Second order stress tensor
φ	[°]	Angle indicating the inclination of principal directions
ϕ	[-]	Porosity

Artificial compressibility for pseudo-unsteady Stokes equations is introduced by considering the linearized balance of mass (**Eq. 5** in main text) for a compressible fluid (**Eq. S5**) where for steady state $\dot{\rho} \rightarrow 0$ holds.

$$\dot{\rho} + \rho_0 \operatorname{div} \mathbf{v} = 0 \quad (\text{S5})$$

The Stokes equations (**Eq. 4** in the main text) are analogously extended (**Eq. S6**) where $\rho \dot{\mathbf{v}} \rightarrow 0$ holds for steady state.

$$\rho \dot{\mathbf{v}} = \mu \operatorname{div}(\operatorname{grad} \mathbf{v}) - \operatorname{grad} p \quad (\text{S6})$$

We apply the dimensionless divergence operator, dimensionless velocity and density to **Equation S5** and receive **Equation S7**:

$$\frac{\mathcal{V}}{\mathcal{L}}(\rho_0^* \dot{\rho}^*) + \frac{\rho_0}{\mathcal{L}} \operatorname{div}(\mathbf{v}^* \mathcal{V}) = 0 \quad \rightarrow \quad (\dot{\rho}^*) \operatorname{div}(\mathbf{v}^*) = 0 \quad (\text{S7})$$

Using the speed of sound for a compression-type wave $c = \sqrt{\frac{K^F}{\rho_0}}$ with its dimensionless form $c = c^* \mathcal{V}$ the constitutive equation for the pressure (**Eq. S4**) is transformed in the same way, yielding (**Eq. S8**):

$$\dot{\rho} = \rho_0 \frac{\dot{p}}{K^F} \rightarrow \dot{\rho} = \frac{\dot{p}}{c^2} \rightarrow \frac{\mathcal{V}}{\mathcal{L}} (\rho_0^* \rho^*)' = \frac{\mathcal{V}(p^* \rho_0^* \mathcal{V}^2)'}{\mathcal{L} c^{*2} \mathcal{V}^2} \rightarrow (\dot{\rho}^*)' = \frac{(\dot{p}^*)'}{c^{*2}} \quad (\text{S8})$$

Plugging Equation S8 into Equation S7, the non-dimensional balance of mass is obtained (Eq. S9):

$$(\dot{p}^*)' = -c^{*2} \text{div}^*(\mathbf{v}^*) \quad (\text{S9})$$

The nondimensional form of the pseudo-unsteady Stokes problem (Eq. S6) yields Equation S10:

$$\frac{\rho_0 \rho^* \mathcal{V}}{\mathcal{L}} (\dot{\mathbf{v}}^* \mathcal{V})' = \frac{\mu}{\mathcal{L}^2} \text{div}^* \text{grad}^*(\mathbf{v}^* \mathcal{V}) - \frac{1}{\mathcal{L}} \text{grad}^*(p^* \rho_0^* \mathcal{V}^2) \rightarrow \rho^* (\dot{\mathbf{v}}^*)' = \frac{1}{\text{Re}} \text{div}^* \text{grad}^*(\mathbf{v}^*) - \text{grad}^*(p^*) \quad (\text{S10})$$

C. DISCRETE EQUATIONS AND FLUID-SOLID BOUNDARY CONDITIONS

Discrete updates: We will briefly present the discrete equations without further details. This is elaborated on in depth in Gerke et al. (2). For velocity and pressure updates one receives (Eq. S11, Eq. S12):

$$v_i^{t+1} = v_i^t + \left\{ \frac{\partial p}{\partial x_i} + \frac{1}{\text{Re}} \left[\left(\frac{\partial^2 v_i}{\partial x_1^2} \right) + \left(\frac{\partial^2 v_i}{\partial x_2^2} \right) + \left(\frac{\partial^2 v_i}{\partial x_3^2} \right) \right] \right\} \Delta t \quad (\text{S11})$$

$$p^{t+1} = p^t - c^2 \left(\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} \right) \Delta t \quad (\text{S12})$$

For the sake of improved readability, we have omitted explicitly indicating that all quantities are dimensionless. Central difference stencils were used, and we refer to the section below for the second order terms.

Fluid-solid boundary treatment: The Taylor expansion around the point x_0 is generally given by the following series (Eq. S13):

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!} (x - x_0)^n = f^{(0)} + f^{(1)}(x - x_0) + \frac{1}{2} f^{(2)}(x - x_0)^2 + \dots \quad (\text{S13})$$

As briefly described in Section 4 for case 2 depicted in Figure 1 in the main text, for the other given cases, the following system of equations can be derived. By solving the given sets of equation systems, the corresponding second-order derivatives $\left(\frac{\partial^2 v_k}{\partial x_i^2} \right)$ in the perpendicular directions to the considered flow velocity direction for $i, j, k = (1,2,3), (2,3,1), (3,1,2)$ can be determined (Eq. S14, Eq. S15, Eq. S16, Eq. S17, Eq. S18, Eq. S19).

$$\text{Case 1: } \left. \begin{aligned} v_{k_1} &\approx v_{k_2} - \frac{1}{2} \frac{\partial v_k}{\partial x_i} + \frac{1}{8} \frac{\partial^2 v_k}{\partial x_i^2} - \frac{1}{48} \frac{\partial^3 v_k}{\partial x_i^3} = 0 \\ v_{k_3} &\approx v_{k_2} + \frac{1}{2} \frac{\partial v_k}{\partial x_i} + \frac{1}{8} \frac{\partial^2 v_k}{\partial x_i^2} + \frac{1}{48} \frac{\partial^3 v_k}{\partial x_i^3} = 0 \end{aligned} \right\} \sim \frac{\partial^2 v_k}{\partial x_i^2} = -8v_{k_2} \quad (\text{S14})$$

$$\text{Case 2: } \left. \begin{aligned} v_{k_1} &\approx v_{k_2} - \frac{1}{2} \frac{\partial v_k}{\partial x_i} + \frac{1}{8} \frac{\partial^2 v_k}{\partial x_i^2} - \frac{1}{48} \frac{\partial^3 v_k}{\partial x_i^3} = 0 \\ v_{k_3} &\approx v_{k_2} + \frac{\partial v_k}{\partial x_i} + \frac{1}{2} \frac{\partial^2 v_k}{\partial x_i^2} + \frac{1}{6} \frac{\partial^3 v_k}{\partial x_i^3} \\ v_{k_4} &\approx v_{k_2} + \frac{3}{2} \frac{\partial v_k}{\partial x_i} + \frac{9}{8} \frac{\partial^2 v_k}{\partial x_i^2} + \frac{9}{16} \frac{\partial^3 v_k}{\partial x_i^3} = 0 \end{aligned} \right\} \sim \frac{\partial^2 v_k}{\partial x_i^2} = \frac{8}{3} v_{k_3} - \frac{16}{3} v_{k_2} \quad (\text{S15})$$

$$\text{Case 3: } \left. \begin{aligned} v_{k_1} &\approx v_{k_3} - \frac{3}{2} \frac{\partial v_k}{\partial x_i} + \frac{9}{8} \frac{\partial^2 v_k}{\partial x_i^2} - \frac{9}{16} \frac{\partial^3 v_k}{\partial x_i^3} = 0 \\ v_{k_2} &\approx v_{k_3} - \frac{\partial v_k}{\partial x_i} + \frac{1}{2} \frac{\partial^2 v_k}{\partial x_i^2} - \frac{1}{6} \frac{\partial^3 v_k}{\partial x_i^3} \\ v_{k_4} &\approx v_{k_3} + \frac{1}{2} \frac{\partial v_k}{\partial x_i} + \frac{1}{8} \frac{\partial^2 v_k}{\partial x_i^2} + \frac{1}{48} \frac{\partial^3 v_k}{\partial x_i^3} = 0 \end{aligned} \right\} \leadsto \frac{\partial^2 v_k}{\partial x_i^2} = \frac{8}{3} v_{k_2} - \frac{16}{3} v_{k_3} \quad (\text{S16})$$

$$\text{Case 4: } \left. \begin{aligned} v_{k_1} &\approx v_{k_2} - \frac{1}{2} \frac{\partial v_k}{\partial x_i} + \frac{1}{8} \frac{\partial^2 v_k}{\partial x_i^2} - \frac{1}{48} \frac{\partial^3 v_k}{\partial x_i^3} = 0 \\ v_{k_3} &\approx v_{k_2} + \frac{\partial v_k}{\partial x_i} + \frac{1}{2} \frac{\partial^2 v_k}{\partial x_i^2} + \frac{1}{6} \frac{\partial^3 v_k}{\partial x_i^3} \\ v_{k_4} &\approx v_{k_2} + 2 \frac{\partial v_k}{\partial x_i} + 2 \frac{\partial^2 v_k}{\partial x_i^2} + \frac{4}{3} \frac{\partial^3 v_k}{\partial x_i^3} \end{aligned} \right\} \leadsto \frac{\partial^2 v_k}{\partial x_i^2} = 2v_{k_3} - 5v_{k_2} - \frac{1}{5} v_{k_4} \quad (\text{S17})$$

$$\text{Case 5: } \left. \begin{aligned} v_{k_1} &\approx v_{k_3} - 2 \frac{\partial v_k}{\partial x_i} + 2 \frac{\partial^2 v_k}{\partial x_i^2} - \frac{4}{3} \frac{\partial^3 v_k}{\partial x_i^3} \\ v_{k_2} &\approx v_{k_3} - \frac{\partial v_k}{\partial x_i} + \frac{1}{2} \frac{\partial^2 v_k}{\partial x_i^2} - \frac{1}{6} \frac{\partial^3 v_k}{\partial x_i^3} \\ v_{k_4} &\approx v_{k_3} + \frac{1}{2} \frac{\partial v_k}{\partial x_i} + \frac{1}{8} \frac{\partial^2 v_k}{\partial x_i^2} + \frac{1}{48} \frac{\partial^3 v_k}{\partial x_i^3} = 0 \end{aligned} \right\} \leadsto \frac{\partial^2 v_k}{\partial x_i^2} = 2v_{k_2} - \frac{1}{5} v_{k_1} - 5v_{k_3} \quad (\text{S18})$$

$$\text{Case 6: } \left. \begin{aligned} v_{k_1} &\approx v_{k_2} - \frac{\partial v_k}{\partial x_i} + \frac{1}{2} \frac{\partial^2 v_k}{\partial x_i^2} - \frac{1}{6} \frac{\partial^3 v_k}{\partial x_i^3} \\ v_{k_3} &\approx v_{k_2} + \frac{\partial v_k}{\partial x_i} + \frac{1}{2} \frac{\partial^2 v_k}{\partial x_i^2} + \frac{1}{6} \frac{\partial^3 v_k}{\partial x_i^3} \end{aligned} \right\} \leadsto \frac{\partial^2 v_k}{\partial x_i^2} = v_{k_1} - 2v_{k_2} + v_{k_3} \quad (\text{S19})$$

D. PERMEABILITY COMPUTATION

For $\text{Re} < 1.0$ the entries of the permeability tensor can be computed using Darcy's law (1), where $h_i = -\frac{\partial p}{\partial x_i} = -p_{,i}$ is the hydraulic gradient (Eq. S20).

$$\mathbf{q} = \frac{1}{\mu} \mathbf{k} \cdot \mathbf{h} \rightarrow q_i \mathbf{e}_i = \frac{1}{\mu} \mathbf{k}_{ij} (\mathbf{e}_i \otimes \mathbf{e}_j) \cdot h_k \mathbf{e}_k = \frac{1}{\mu} \mathbf{k}_{ik} h_k \mathbf{e}_i \quad \text{with} \quad q_i = \frac{1}{A_i} \int_{\partial \mathcal{B}} v_i d\bar{A}_i \quad (\text{S20})$$

The numerical experiments must be performed to determine the nine entries in the coefficient matrix of the second order permeability tensor. Thereby, the following pressure gradients are applied for the (Eq. S21) different cases, and we measure three fluxes q_i for each case.

$$\begin{aligned} a) \quad & h_1 \neq 0 \wedge h_2 = h_3 = 0 \\ b) \quad & h_2 \neq 0 \wedge h_1 = h_3 = 0 \\ c) \quad & h_3 \neq 0 \wedge h_1 = h_2 = 0 \end{aligned} \quad (\text{S21})$$

By comparing the coefficients for the three equations for the flow q_i (Eq. S20, right) we receive (Eq. S22):

$$q_i = -\frac{1}{\mu} k_{ik} h_k \rightarrow \begin{aligned} i) \quad & q_1 = -\frac{1}{\mu} [k_{11} h_1 + k_{12} h_2 + k_{13} h_3] \\ ii) \quad & q_2 = -\frac{1}{\mu} [k_{21} h_1 + k_{22} h_2 + k_{23} h_3] \\ iii) \quad & q_3 = -\frac{1}{\mu} [k_{31} h_1 + k_{32} h_2 + k_{33} h_3] \end{aligned} \quad (\text{S22})$$

The following nine equations (Eq. S23) arise from the constraints (a–c) provided in Equation S21:

$$\begin{aligned}
 a) \quad q_1 &= -\frac{1}{\mu} k_{11} h_1 & q_2 &= -\frac{1}{\mu} k_{21} h_1 & q_3 &= -\frac{1}{\mu} k_{31} h_1 \\
 b) \quad q_1 &= -\frac{1}{\mu} k_{12} h_2 & q_2 &= -\frac{1}{\mu} k_{22} h_2 & q_3 &= -\frac{1}{\mu} k_{32} h_2 \\
 c) \quad q_1 &= -\frac{1}{\mu} k_{13} h_3 & q_2 &= -\frac{1}{\mu} k_{23} h_3 & q_3 &= -\frac{1}{\mu} k_{33} h_3
 \end{aligned} \tag{S23}$$

This results in nine equations for nine unknown entries of the coefficient matrix of the second order permeability tensor. Numerically determined, one obtains slightly different values for two corresponding secondary diagonal elements. These are therefore averaged $k_{12} = k_{21} = \frac{1}{2}(k_{12} + k_{21})$. The same procedure is adopted for k_{13} , k_{31} and k_{23} , k_{32} .

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