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Analytical benchmark solutions for nanotube flows with variable viscosity

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Three-dimensional Stokes equations with variable viscosity in cylindrical coordinates are considered. This case is natural for flow through a nanotube in biological applications. We obtain exact particular solutions – a benchmark for numerical approache.

Keywords: Stokes flow, variable viscosity, multigrid methods, benchmark solutions.

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1. Introduction

Flow through nanotubes are intensively investigated, particularly due to its biological applications, e.g., as a transport channel for some compounds into the cell (see, e.g., [1]). Although there is no general approach in nanohydrodynamics [2-6], the Stokes approximation (with variable viscosity) is available in many cases. We consider the axisymmetric case, which is natural for the nanotube flow. Biologists need a reliable computational approach to describe and predict the mass transport through a nanotube "to" and "from" the cell. There are several computational schemes for solution of the Stokes and continuity equations, but in the case of strongly varying viscosity, these schemes are plagued by difficulties. One would like to have an instrument for testing of these algorithms. One convenient method is to suggest benchmark solutions for some particular cases [7-9]. In this paper, such a benchmark solution is constructed for the axisymmetric case. It is interesting to note that the same mathematical problem appears in geophysics [10, 11].

This paper deals with the Stokes and continuity equations for the case of variable viscosity and density having the following form:

$$(\nabla \cdot \sigma) = -\rho G \quad , \tag{1}$$

$$\nabla(\rho v) = 0, \tag{2}$$

where v is velocity, η is a dynamic viscosity, σ is the total stress tensor, p is a pressure, G is a gravitational force. We consider equations (1), (2) in cylindrical coordinates (r, φ, z) and construct a solution for the case when the variables depend only on the radius r.

2. Benchmark solutions

We construct particular solutions of the system of Stokes and continuity equations for specific density and viscosity distributions: $\eta = \eta(r)$, $\rho = \rho(r)$. Let $v_r = v_r(r)$, $v_\varphi = v_\varphi(r)$, $v_z = v_z(r)$, $P = P(r)$, $\eta = \eta(r)$, $\rho = \rho(r)$, $G = G(r)$. Then equation (1) simplifies considerably:

$$2\eta\frac{1}{r}v_r^{\cdot} + 2\eta' v_r^{\cdot} + 2\eta v_r^{\cdot\cdot} - 2\eta\frac{1}{r^2}v_r - P' = -\rho G_r \tag{3}$$

$$\eta' v_\varphi^{\cdot} - \frac{1}{r}\eta' v_\varphi + \eta v_\varphi^{\cdot\cdot} + \frac{1}{r}\eta v_\varphi^{\cdot} - \eta\frac{1}{r^2}v_\varphi = -\rho G_\varphi \tag{4}$$

$$\eta\frac{1}{r}v_z^{\cdot} + \eta' v_z^{\cdot} + \eta v_z^{\cdot\cdot} = -\rho G_z. \tag{5}$$

The continuity equation takes the form:

$$\rho\frac{1}{r}v_r + \rho' v_r + \rho v_r^{\cdot} = 0. \tag{6}$$

In this case, we obtain the following solutions of equations (1), (2):

$$\begin{aligned} &v_r = \tfrac{c}{r\rho}, \quad v_\varphi = c_1 f(r) + c_2 r + C_1(r) f(r) + C_2(r) r, \\ &v_z = -\int_1^r \tfrac{1}{\eta r_2}\Big(\int_1^{r_2} r_1 \rho G_z dr_1 + c_1\Big) dr_2 + c_2, \end{aligned} \tag{7}$$

$$P(r) = \int (\rho G_r + 2\eta\frac{1}{r}v_r^{\cdot} + 2\eta' v_r^{\cdot} + 2\eta v_r^{\cdot\cdot} - 2\eta\frac{1}{r^2}v_r)dr, \tag{8}$$

where

$$f(r) = \exp\Big(\int_1^r \Big(\frac{1}{r_2} + \frac{1}{\eta r_2^3}\frac{1}{\int_1^{r_2}\frac{1}{\eta r_1^3}dr_1 + C}\Big)dr_2\Big),$$

$$C_1(r) = \int \frac{r\rho G_\varphi}{\eta(f - f'r)}dr, \quad C_2(r) = -\int \frac{f\rho G_\varphi}{\eta(f - f'r)}dr.$$

Formulas (7), (8) gives us the solution of equations (1), (2). Derivation of the solution is presented in Appendix A in detail.

3. Multigrid method

In this work, we derive a procedure of multigrid method for solving the Stokes equations with variable viscosity in cylindrical coordinates. The analogous algorithm for the Cartesian coordinates was described in [10]. We derive a similar scheme for cylindrical coordinates.

As usual, the multigrid method algorithm contains three steps: 1) smoothing operation 2) restriction operation 3) prolongation operation. Cylindrical coordinates are orthogonal coordinates, thus the implementation of the prolongation and restriction operations in our method is not different from that in the case of the Cartesian coordinates. As for the smoothing operation, it differs. This procedure is described in Appendix B in detail.

The scheme for algorithm testing is as follows. Let us consider some particular analytical solutions (7), (8): $v_r = -\frac{1}{r}$, $v_\varphi = r^2$, $v_z = -\frac{1}{10}\rho G_z r^5 - \frac{1}{3}r^3$, $P(r) = \rho G_r r + 1.2\frac{1}{r^2}$ in the domain $1 \leqslant r \leqslant 2$, $0 \leqslant \phi \leqslant 1$, $0 \leqslant z \leqslant 1$ ($\rho = const$, $G_r = 10$, $G_\varphi = 0$, $G_z = 10$, $\eta = r^{-3}$). We calculate the values for velocity and pressure given by our analytical solution and take these values as the boundary conditions for the numerical algorithm. The deviation of the numerical solution values from the analytical solution is related to the error of the multigrid scheme. The dependence of the relative error on the grid step for the multigrid scheme is shown in Figure.1. Positive curve slopes indicate a convergence for the algorithm.

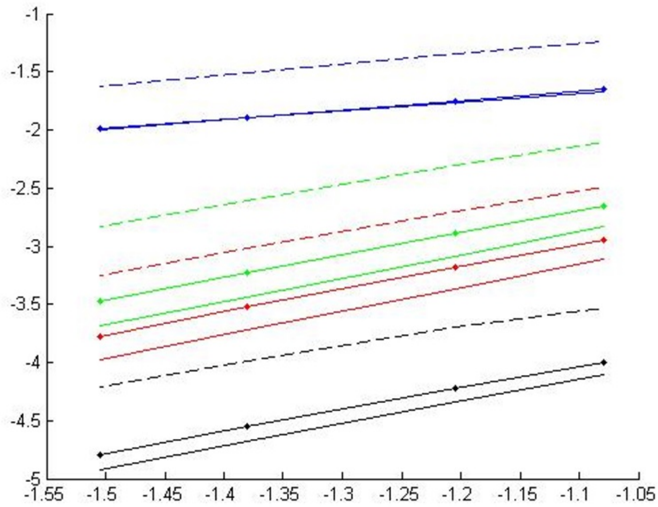

FIG. 1. Error norm via the grid resolution in logarithmic scale: blue lines-pressure, red lines- v_r , black lines - v_φ , green lines - v_z; solid lines - L_1-error, dashed lines- L_∞ -error, solid dotted lines- L_2-error

Appendix A. Derivation of the Stokes equations solution

Integration of (6) gives us:

$$v_r = \frac{c}{r\rho}. \tag{9}$$

Substitution of (9) in (3) gives us the expression for pressure:

$$P(r) = \int (\rho G_r + 2\eta\frac{1}{r}v_r' + 2\eta' v_r' + 2\eta v_r'' - 2\eta\frac{1}{r^2}v_r)dr. \tag{10}$$

Consider equation (4). Simple transformation gives us:

$$v_\varphi'' + v_\phi'(\frac{\eta'}{\eta} + \frac{1}{r}) - v_\phi(\frac{1}{r}\frac{\eta'}{\eta} + \frac{1}{r^2}) = \frac{-\rho G_\varphi}{\eta} \tag{11}$$

We seek a solution of (11) in the form $v_\varphi(r) = v_{\varphi 0}(r) + v_{\varphi 1}(r)$, where $v_{\varphi 0}(r)$ is particular solution of (11) and $v_{\varphi 1}(r)$ is the general solution of the corresponding homogeneous equation:

$$v_\varphi'' + v_\varphi'(\frac{\eta'}{\eta} + \frac{1}{r}) - v_\varphi(\frac{1}{r}\frac{\eta'}{\eta} + \frac{1}{r^2}) = 0. \tag{12}$$

Let us make a replacement:

$$z = \frac{v_\varphi'}{v_\varphi} \tag{13}$$

in (12). It transforms into the first-order equation:

$$z' + z(\frac{\eta'}{\eta} + \frac{1}{r}) + z^2 - \frac{1}{r}\frac{\eta'}{\eta} - \frac{1}{r^2} = 0. \tag{14}$$

If one makes the substitution $z = \frac{1}{\eta r}y$, where $y = y(r)$ then (14) transforms into the Riccati equation:

$$y' + y^2\frac{1}{\eta r} - \eta' - \frac{\eta}{r} = 0. \tag{15}$$

Function $y = \eta$ is a particular solution of (15). Keeping this in mind, we seek the solution in the form $y = u + \eta$. For function $u = u(r)$ one obtains the Bernoulli equation:

$$u' = -2\frac{1}{r}u - \frac{1}{\eta r}u^2. \tag{16}$$

Note that $u(r) = 0$ is a solution. We seek a non-trivial solution of (16) in the form $u = \frac{1}{r^2}q$, where $q = q(r)$. The equation simplifies:

$$q' + \frac{1}{\eta r^3}q^2 = 0,$$

giving us:

$$q = \frac{1}{\int \frac{1}{\eta r^3}dr}$$

Coming back to (12), we get:

$$\frac{v'_\varphi}{v_\varphi} = \frac{1}{\eta r}(\eta + \frac{1}{r^2}\frac{1}{\int \frac{1}{\eta r^3}dr})$$

After integration, one obtains:

$$\ln(|v_\varphi|) = \int_1^r (\frac{1}{r_2} + \frac{1}{\eta r_2^3}\frac{1}{\int_1^{r_2} \frac{1}{\eta r_1^3}dr_1 + c_{11}})dr_2 + c_{21}$$

Solution $u(r) = 0$ of (16) leads to the following solution of (12):

$$v_\varphi = cr$$

As a result, we obtain the general solution of (12) in the following form:

$$v_{\varphi 1}(r) = c_1 f(r) + c_2 r,$$

where $f(r) = \exp(\int_1^r (\frac{1}{r_2} + \frac{1}{\eta r_2^3}\frac{1}{\int_1^{r_2} \frac{1}{\eta r_1^3}dr_1 + C})dr_2)$.

We seek a particular solution of equation (11) by the Lagrange method in the form $v_{\varphi 0}(r) = C_1(r)f(r) + C_2(r)r$.

Here $C_1(r)$, $C_2(r)$ satisfy the system of equation:

$$\begin{array}{l} C_1' f(r) + C_2' r = 0 \\ C_1' f'(r) + C_2' = \frac{-\rho G_\varphi}{\eta} \end{array}.$$

Correspondingly, $C_1(r) = \int \frac{r\rho G_\varphi}{\eta(f - f'r)}dr$, $C_2(r) = -\int \frac{f\rho G_\varphi}{\eta(f - f'r)}dr$

As a result, we come to the following solution of equation (4):

$$v_\varphi(r) = c_1 f(r) + c_2 r + C_1(r)f(r) + C_2(r)r, \tag{17}$$

we let $v_z = w(r)$, equation (8) takes the form:

$$w' + (\frac{\eta'}{\eta} + \frac{1}{r})w = -\frac{\rho}{\eta}G_z \tag{18}$$

If one makes the substitution $w = \varpi\frac{1}{\eta r}$, where $\varpi = \varpi(r)$, then (11) transforms into equation:

$$\varpi'\frac{1}{\eta r} = -\frac{\rho}{\eta}G_z$$

Integration gives us:

$$w = -\frac{1}{\eta r}(\int\limits_1^r r_1 \rho G_z dr_1 + c_1),$$

As a result, we get the following expression for the velocity component:

$$v_z = -\int\limits_1^r \frac{1}{\eta r_2}(\int\limits_1^{r_2} r_1 \rho G_z dr_1 + c_1)dr_2 + c_2. \quad (19)$$

Appendix B. Gauss-Seidel smoother

Smoothing operation can be implemented on the basis of Gauss-Seidel iterations. The respective iterative pressure and velocity update schemes for a regularly spaced grid can be derived:

$$P^{new}_{(i,j,l)} = P_{(i,j,l)} + \eta_{n(i,j,l)} \Delta R^{continuity}_{i,j,l} \theta^{continuity}_{relaxation} \quad (20)$$

$$\Delta R^{continuity}_{i,j,l} = R^{continuity}_{i,j,l} - \frac{v_r}{r} - \frac{\partial v_r}{\partial r} - \frac{1}{r}\frac{\partial v_\varphi}{\partial \varphi} - \frac{\partial v_z}{\partial z}, \quad (21)$$

$$v^{new}_{r(i,j,l)} = v_{r(i,j,l)} + \frac{\Delta R^{r-Stokes}_{i,j,l}}{C_{v_r(i,j,l)}} \theta^{Stokes}_{relaxation} \quad (22)$$

$$v^{new}_{\phi(i,j,l)} = v_{\varphi(i,j,l)} + \frac{\Delta R^{\varphi-Stokes}_{i,j,l}}{C_{v_\varphi(i,j,l)}} \theta^{Stokes}_{relaxation} \quad (23)$$

$$v^{new}_{z(i,j,l)} = v_{z(i,j,l)} + \frac{\Delta R^{z-Stokes}_{i,j,l}}{C_{v_z(i,j,l)}} \theta^{Stokes}_{relaxation} \quad (24)$$

where $\theta^{continuity}_{relaxation}, \theta^{Stokes}_{relaxation}$ are relaxation parameters. $C_{v_r(i,j,l)}$, $C_{v_\varphi(i,j,l)}$,$C_{v_z(i,j,l)}$ is the coefficients at $v_{r(i,j,l)} v_{\varphi(i,j,l)}$, $v_{z(i,j,l)}$ in Stokes equations (1). For models with variable viscosity, the respective residuals in Eqs.(22)–(24) become:

$$\Delta R^{r-Stokes}_{i,j,l} = R^{r-Stokes}_{i,j,l} - \frac{\partial \tau_{rr}}{\partial r} - \frac{\tau_{rr} - \tau_{\varphi\varphi}}{r} - \frac{1}{r}\frac{\partial \tau_{r\varphi}}{\partial \varphi} - \frac{\partial \tau_{rz}}{\partial z} + \frac{\partial P}{\partial r}, \quad (25)$$

$$\Delta R^{\varphi-Stokes}_{i,j,l} = R^{\varphi-Stokes}_{i,j,l} - \frac{\partial \tau_{r\varphi}}{\partial r} - \frac{2\tau_{r\varphi}}{r} - \frac{1}{r}\frac{\partial \tau_{\varphi\varphi}}{\partial \varphi} - \frac{\partial \tau_{\varphi z}}{\partial z} + \frac{1}{r}\frac{\partial P}{\partial \varphi}, \quad (26)$$

$$\Delta R^{z-Stokes}_{i,j,l} = R^{z-Stokes}_{i,j,l} - \frac{\partial \tau_{rz}}{\partial r} - \frac{\tau_{rz}}{r} - \frac{1}{r}\frac{\partial \tau_{\varphi z}}{\partial \varphi} - \frac{\partial \tau_{zz}}{\partial z} + \frac{\partial P}{\partial z} \quad (27)$$

where τ is a deviatoric stress tensor.

B.1 Discretization of the continuity equation

Fig. 2 shows an elementary volume (cell) of a 3D staggered grid that can be used for discretization. Using the stencil with six velocity nodes around a cell (Fig.2), equation (21) takes the form:

$$\Delta R^{continuity}_{i,j,l} = R^{continuity}_{i,j,l} - \frac{1}{r_j + \Delta r/2} \frac{v_{r(i+1,j+1,l+1)} + v_{r(i+1,j,l+1)}}{2} - \frac{v_{r(i+1,j+1,l+1)} - v_{r(i+1,j,l+1)}}{\Delta r} -$$
$$- \frac{1}{r_j + \Delta r/2} \frac{v_{\varphi(i+1,j+1,l+1)} - v_{\varphi(i,j+1,l+1)}}{\Delta \varphi} - \frac{v_{z(i+1,j+1,l+1)} - v_{z(i+1,j+1,l)}}{\Delta z}$$

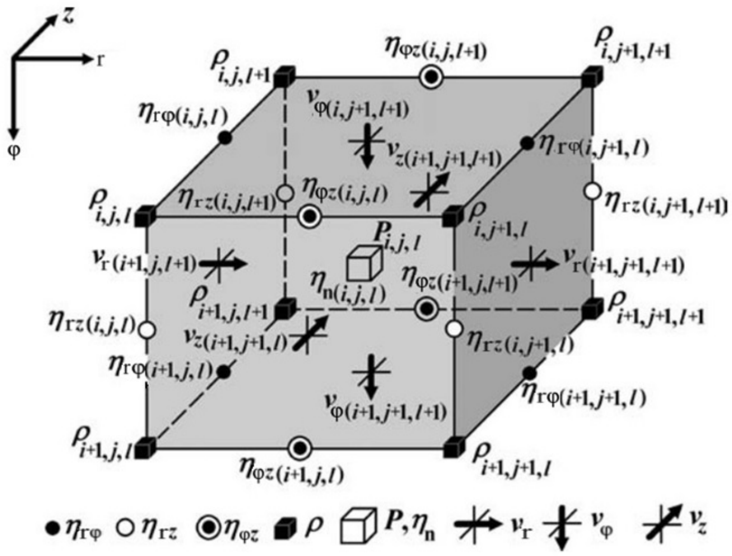

FIG. 2. Indexing of different variables for a 3D staggered grid

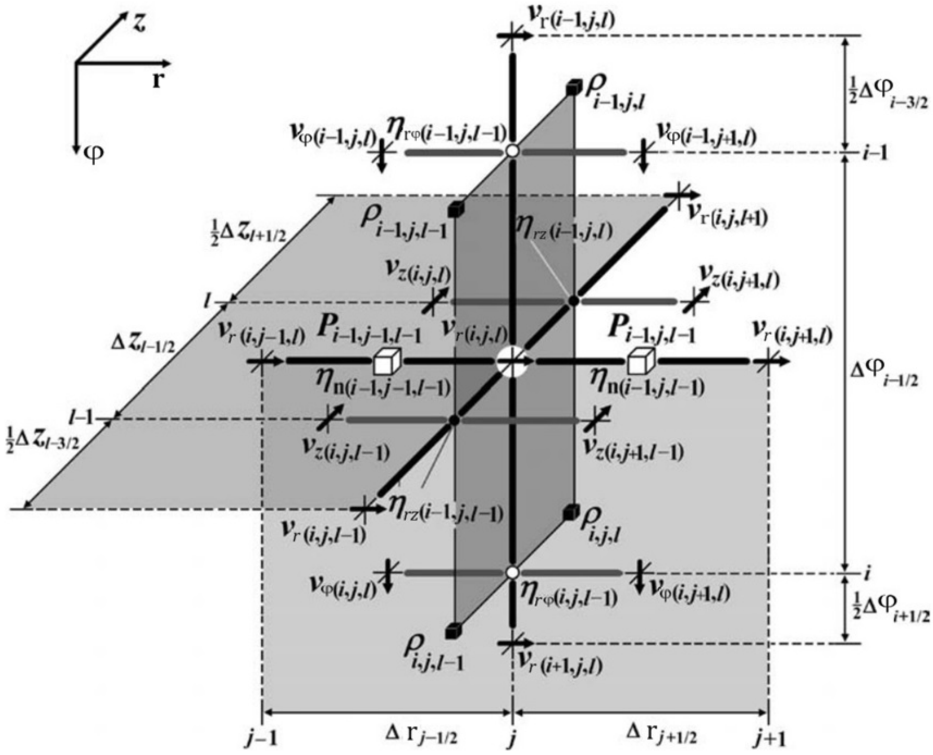

FIG. 3. Stencil of a 3D staggered grid used for the discretization of the r-Stokes equation with variable viscosity

B.2 Discretization of Stokes equations

An example of stencil for the discretization of the r-Stokes equation is shown in Fig.3. For terms in equations (22), (25), we obtain the following discretization:

1. Pressure derivative:

$$\frac{\partial P}{\partial r} = \frac{P_{(i-1,j,l-1)} - P_{(i-1,j-1,l-1)}}{\Delta r}$$

Discretization for terms which contain deviatoric stress tensor components:

2.

$$(\frac{\partial \tau_{rr}}{\partial r})_{i,j,l} = (\frac{\partial}{\partial r}(2\eta\frac{\partial v_r}{\partial r}))_{i,j,l} = 2\frac{1}{\Delta r}(\eta_{(i-1,j,l-1)}\frac{v_{r(i,j+1,l)} - v_{r(i,j,l)}}{\Delta r} - \eta_{(i-1,j-1,l-1)}\frac{v_{r(i,j,l)} - v_{r(i,j-1,l)}}{\Delta r})$$

3.

$$(\tau_{rr})_{i,j,l} = (2\eta\frac{\partial v_r}{\partial r})_{i,j,l} = (\eta_{n(i-1,j,l-1)} + \eta_{n(i-1,j-1,l-1)})\frac{v_{r(i,j+1,l)} - v_{r(i,j-1,l)}}{2\Delta r}$$

4.

$$(\tau_{\varphi\varphi})_{i,j,l} = (2\eta(\tfrac{1}{r}\tfrac{\partial v_\varphi}{\partial \varphi} + \tfrac{v_r}{r}))_{i,j,l} = \tfrac{1}{r_j}(\eta_{n(i-1,j,l-1)} + \eta_{n(i-1,j-1,l-1)})(\tfrac{1}{\Delta\varphi}(\tfrac{v_{\varphi(i,j+1,l)}+v_{\varphi(i,j,l)}}{2} - \\ - \tfrac{v_{\varphi(i-1,j+1,l)}+v_{\varphi(i-1,j,l)}}{2}) + v_{r(i,j,l)})$$

5.

$$(\tfrac{\partial \tau_{r\varphi}}{\partial \varphi})_{i,j,l} = (\tfrac{\partial}{\partial\varphi}(\eta(\tfrac{1}{r}\tfrac{\partial v_r}{\partial\varphi} + \tfrac{\partial v_\varphi}{\partial r} - \tfrac{v_\varphi}{r})))_{i,j,l} = \tfrac{1}{\Delta\varphi}(\eta_{r\varphi(i,j,l-1)}(\tfrac{1}{r_j}\tfrac{v_{r(i+1,j,l)}-v_{r(i,j,l)}}{\Delta\varphi} + \tfrac{v_{\varphi(i,j+1,l)}-v_{\varphi(i,j,l)}}{\Delta r} \\ - \tfrac{1}{r_j}\tfrac{v_{\varphi(i,j+1,l)}+v_{\varphi(i,j,l)}}{2}) - \eta_{r\varphi(i-1,j,l-1)}(\tfrac{1}{r_j}\tfrac{v_{r(i,j,l)}-v_{r(i-1,j,l)}}{\Delta\varphi} + \tfrac{v_{\varphi(i-1,j+1,l)}-v_{\varphi(i-1,j,l)}}{\Delta r} - \tfrac{1}{r_j}\tfrac{v_{\varphi(i-1,j+1,l)}+v_{\varphi(i-1,j,l)}}{2}))$$

6.

$$(\tfrac{\partial \tau_{rz}}{\partial z})_{i,j,l} = (\tfrac{\partial}{\partial z}(\eta(\tfrac{\partial v_z}{\partial r} + \tfrac{\partial v_r}{\partial z})))_{i,j,l} = \tfrac{1}{\Delta z}\eta_{rz(i-1,j,l)}(\tfrac{v_{z(i,j+1,l)}-v_{z(i,j,l)}}{\Delta r} + \tfrac{v_{r(i,j,l+1)}-v_{r(i,j,l)}}{\Delta z}) - \\ -\eta_{rz(i-1,j,l-1)}(\tfrac{v_{z(i,j+1,l-1)}-v_{z(i,j,l-1)}}{\Delta r} + \tfrac{v_{r(i,j,l)}-v_{r(i,j,l-1)}}{\Delta z}).$$

Discretization for coefficient $C_{v_r(i,j,l)}$ in equation (16) takes the form:

$$C_{v_r(i,j,l)} = -2\tfrac{\eta_{n(i-1,j,l-1)}+\eta_{n(i-1,j-1,l-1)}}{\Delta r^2} - \tfrac{\eta_{n(i-1,j,l-1)}+\eta_{n(i-1,j-1,l-1)}}{r_j^2} - \\ -\tfrac{1}{r_j^2}\tfrac{\eta_{r\varphi(i,j,l-1)}+\eta_{r\varphi(i-1,j,l-1)}}{\Delta\varphi^2} - \tfrac{\eta_{rz(i-1,j,l)}+\eta_{rz(i-1,j,l-1)}}{\Delta z^2}$$

Discretization for the φ-Stokes and z-Stokes equations can be constructed and indexed analogously.

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