1 General information

This software is a script compilation for FreeFem++ to solve interface cell problems and arrive with coefficients in boundary condition (BC) between porous medium and free fluid. This module gives the possibility to compute the coefficients for BC in two-dimensions (2D) for porous case. If you find this software useful, please cite the corresponding publication <DOI:10.1017/jfm.2016.838> (open access) This software is also suitable to determine coefficients in TR model (improved accuracy over the original work), which is available in as a pre-print <arXiv:1812.09401>.

The contents of this module are listed below.

```
src/2D_MSE_bc_solver.edp        - script to solve for BC coefficients tensor
src/2D_MSE_solver.edp           - script to solve a Cavity problem with
                                  developed boundary conditions
doc/2D_MSE_bc_velocity.pdf      - this document
```

Two additional .idp files are provided but not described in detail. In this document we explain the key elements of the software, parameters of the simulation, and implemented variational formulation.

2 Solver for interface tensors K and L

2.1 Structure of the simulation script

The simulation script take following input:

1. geometry of the interface cell (through predefined presets or custom definition);
2. interface location ($intfShft$);
3. extent of the cell (set by number of structures $Nstr$);
4. solid volume fraction ($thetas$) and other structure parameters;

The geometry and mesh (resolution controlled by parameters n – segments per unit length –, $nIntf$ – refinement at interface –, and nS – refinement at solid structures) currently are generated within the software, but could be generated using some other tool and read in.

In the code, there are three presets for geometry generation defined, “cylinder” (isotropic cylinder configuration), “laycyl” (layered cylinder configuration) and “ellipse” (tilted ellipse configuration). The first one corresponds to the original work <DOI:10.1017/jfm.2016.838>, while the second two were in addition considered in the improved publication <arXiv:1812.09401>. The switching between the presets are implemented using the macro “geomPreset” as

```
48 macro geomPreset()cylinder// EOM
49 real thetas = 0.25;
```

Note that there can be no white space between name defined by the macro and end-of-macro (comment symbols "//"). The geometry generation relies on use of macros and IFMACRO statement, introduced in relatively recent FreeFEM++ version, 3.51 and above.

Assertion is carried out to ensure that interface is not slicing the upper structure (line 81). Additionally, the classical permeability problem of the interior is defined and solved in lines 86–116 for getting appropriate boundary conditions for the interface cell (see main paper), the results are saved in separate finite element functions.

The result of the simulation script is tensor fields at the full interface cell. The plane average result is outputted in text files, while resulting boundary condition coefficients are outputted to the console.

2.2 Variational formulation

The developed software solve coupled systems of Stoke's equations. By fixing indices k, l, we set $u_i^{K^\pm} = K_{ik}^\pm$, $u_i^{L^\pm} = L_{ikl}^\pm$, $p^{K^\pm} = A_k^\pm$ and $p^{L^\pm} = B_{kl}^\pm$. Then the governing equations take form (see paper<DOI:10.1017/jfm.2016.838> for all details)

$$-p^{K^+}_{,i} + u^{K^+}_{i,jj} = 0, \qquad -p^{L^+}_{,i} + u^{L^+}_{i,jj} = 0, \tag{1}$$

$$u^{K^+}_{i,i} = 0, \qquad u^{L^+}_{i,i} = 0, \tag{2}$$

$$u_i^{K^+}\Big|_{\Gamma_C} = 0, \qquad u_i^{L^+}\Big|_{\Gamma_C} = 0, \tag{3}$$

$$u_i^{K^-}\Big|_{\Gamma_I} = u_i^{K^+}\Big|_{\Gamma_I}, \qquad u_i^{L^-}\Big|_{\Gamma_I} = u_i^{L^+}\Big|_{\Gamma_I}, \tag{4}$$

$$[-p^{K^+}\delta_{ij} + 2\,\varepsilon_{ij}\left(u^{K^+}\right)]\Big|_{\Gamma_I} n_j = \qquad [-p^{L^+}\delta_{ij} + 2\,\varepsilon_{ij}\left(u^{L^+}\right)]\Big|_{\Gamma_I} n_j = \tag{5}$$

$$= [-p^{K^-}\delta_{ij} + 2\,\varepsilon_{ij}\left(u^{K^-}\right)]\Big|_{\Gamma_I} n_j, \qquad = [-p^{L^-}\delta_{ij} + 2\,\varepsilon_{ij}\left(u^{L^-}\right)]\Big|_{\Gamma_I} n_j - \delta_{ik}n_l, \tag{6}$$

$$-p^{K^-}_{,i} + u^{K^-}_{i,jj} = -\delta_{ik}, \qquad -p^{L^-}_{,i} + u^{L^-}_{i,jj} = 0, \tag{7}$$

$$u^{K^-}_{i,i} = 0, \qquad u^{L^-}_{i,i} = 0, \tag{8}$$

$$u_i^{K^-}\Big|_{\Gamma_C} = 0, \qquad u_i^{L^-}\Big|_{\Gamma_C} = 0. \tag{9}$$

Structure of both set of equation systems is exactly the same, the only difference lies in volume forcing and stress boundary condition. Without loosing generality, we proceed by showing how to solve problems for K. In order to simplify notation, we skip the K in equations. In order to solve these problems, we define test functions $\hat{u}_i^\pm$ and $\hat{p}^\pm$ and $\hat{\lambda}$ for velocity and pressure To arrive with weak formulation, we multiply equations with test function and employ integration

by parts for fluid stresses, designated by $\Sigma_{ij}^{\pm} = -p^{\pm}\delta_{ij} + 2\varepsilon_{ij}\left(u^{\pm}\right)$, to obtain

$$-\int_{\Omega} \Sigma_{ij}^{+}\hat{u}_{i,j}^{+}\, d\Omega + \int_{\partial\Omega} \Sigma_{ij}^{+} n_j \hat{u}_i^{+}\, dS = 0, \tag{10}$$

$$\int_{\Omega} u_{i,i}^{+}\hat{p}^{+}\, d\Omega = 0, \tag{11}$$

$$-\int_{\Omega} \Sigma_{ij}^{-}\hat{u}_{i,j}^{-}\, d\Omega + \int_{\partial\Omega} \Sigma_{ij}^{-} n_j \hat{u}_i^{-}\, dS = -\int_{\Omega} \delta_{ik}\hat{u}_i^{-}\, d\Omega, \tag{12}$$

$$\int_{\Omega} u_{i,i}^{-}\hat{p}^{-}\, d\Omega = 0, \tag{13}$$

for governing equations. This weak formulation is implemented using problem statements (lines 153–159 and 189–195). The surface forcing for the slip problem is enforced using surface integral on the interior boundary.

3 Solver for led driven cavity flow over porous medium

The simulation script take following input:

1. geometry of the flow problem, both free fluid and porous medium, number of grid points n per unit length;
2. scale separation parameter $epsP$ and volume fraction $thetas$;
3. interface location (yif);
4. results from interface cell (tensors K and L);
5. Upper wall velocity $Udrv$.

The domain consists of free fluid domain Ω_f and porous medium domain Ω_p, encompassed by boundaries at interface Γ_{if}, upper wall Γ_{f2} and side walls Γ_{f13} of free fluid, and lower wall Γ_{p4} and side walls Γ_{p13} of porous domain. Within these two domains, we solve equation system

$$-p_{,i} + \epsilon u_{i,jj} = 0 \qquad \text{in } \Omega_f, \qquad u_i|_{\Gamma_{f13}} = 0, \quad u_1|_{\Gamma_{f2}} = Udrv, \quad u_2|_{\Gamma_{f2}} = 0, \tag{14}$$

$$u_{i,i} = 0 \qquad \text{in } \Omega_f, \qquad u_1|_{\Gamma_{if}} = -K_{1j}\frac{\tilde{p}_{,j}}{\epsilon} + L_{1ij}\left(u_{i,j} + u_{j,i}\right), \tag{15}$$

$$u_2|_{\Gamma_{if}} = -K_{2j}\frac{\tilde{p}_{,j}}{\epsilon} + L_{2ij}\left(u_{i,j} + u_{j,i}\right), \tag{16}$$

$$\tilde{p}_{,jj} = 0 \qquad \text{in } \Omega_p, \qquad \tilde{p}|_{\Gamma_{if}} = p, \quad \tilde{p}_{,1}|_{\Gamma_{p13}} = 0, \quad \tilde{p}_{,2}|_{\Gamma_{p4}} = 0. \tag{17}$$

The Darcy flow in the interior is expressed using the Darcy law with constant isotropic permeability K_{drc}

$$\tilde{u}_i = -K_{drc}\frac{\tilde{p}_{,i}}{\epsilon}. \tag{18}$$

For the final remark, we have observed that construction of Lagrange multipliers is different. Before we saw that transpose operation was always sufficient (and required) for accurate solution. However, in this case, one has to explicitly define that forcing from velocity boundary condition acts only on velocities (and not on derivatives of velocity or pore pressure), while pressure boundary condition for pore pressure equation acts only as forcing in the pore pressure equation. Otherwise, the weak form and solver is constructed exactly as described in the previous section.