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 or textured 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 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 pre-sets or custom definition);
2. interface location (y_i);
3. extent of the cell (set by number of structures $Nstr$);
4. solid volume fraction ($thetas$) and other structure parameters;

Currently the geometry is generated within the FreeFem++. The mesh resolution is controlled by parameters n – segments per unit length –, $nIntf$ – refinement at interface – and nS – refinement at solid structures.

Currently, there are two pre-sets defined for the textured surfaces and three pre-sets defined for porous surfaces. To switch between textured and porous surfaces, one has to modify the macro

```
46 macro Type()textured// EOM
```

which can take values “textured” or “porous”. Two textured pre-sets available are “tricav” and “rctcav”, which have been tested in <arXiv:1812.09401>. The porous pre-sets are “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 <arXiv:1812.09401>. The switching between the presets are implemented using the macro "geomPreset" as

```
47 macro geomPreset()rctcav// EOM
48 real wdth = 0.5;
49 real dpth = 0.5;
```

followed by the needed geometrical parameters. 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. More examples of geometry definition can be found in example file "examples_geomDef.edp". The convention of all geometries is that the upper most solid point has coordinate $y = 0$. For structures, where the upper surface has planar component, it is possible to set interface coordinate to $y_i = 0$. For curved surfaces it is not possible do to practical reasons. The zero interface location is indicated with the macro

```
60 macro itfFlag()zero// EOM // Interface flag, "above" or "zero"
```

Assertion is carried out for proper definition of the interface location (lines 63–64). Additionally, for the porous set-ups, the classical interior permeability problem is defined and solved in include file "include_interK.idp" and used in the main solver, see lines 76–82. The solution is later used for getting appropriate boundary conditions for the interface cell see <DOI:10.1017/jfm.2016.838>), the results are stored 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. The fields are post-processed according to <DOI:10.1017/jfm.2016.838> and <arXiv:1812.09401>; resulting boundary condition coefficients are outputted to the console and saved to text files.

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)

$$-p_{,i}^{K^+} + u_{i,jj}^{K^+} = 0, \qquad -p_{,i}^{L^+} + u_{i,jj}^{L^+} = 0, \tag{1}$$

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

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

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

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

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

$$-p_{,i}^{K^-} + u_{i,jj}^{K^-} = -\delta_{ik}, \qquad -p_{,i}^{L^-} + u_{i,jj}^{L^-} = 0, \tag{7}$$

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

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

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. We also do not implement the forcing directions for the L problem which are zero by construction. In order to simplify notation, we skip the K in equations. To solve these problems, we define test functions $\hat{u}_i^\pm$ and $\hat{p}^\pm$ 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 $\Sigma_{ij}^\pm = -p^\pm\delta_{ij} + 2\varepsilon_{ij}\,(u^\pm)$, 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 113–124 and 161–166). 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}

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

The weak form for Stokes equations are obtained as explained in the previous section, while for the Darcy region the weak for is obtained as for a standard Poisson equation. The boundary conditions at the coupled interface are ensured by help of Lagrange multipliers, i.e., additional test function $\hat{\lambda}$ is introduced and boundary conditions are multiplied with the function and integrated over the surface. The feedback to governing equations has been empirically determined. The forcing term from boundary conditions of velocity acts only on velocities (and not on derivatives of velocity or pore pressure), while forcing from pressure boundary condition for pore pressure equation acts only in the pore pressure equation. We have also empirically determined the resolution for Langrange multiplier space and the finite element order, see the main simulation file.