XXXVI Ibero-Latin American Congress on Computational Methods in Engineering
CILAMCE
Rio de Janeiro, 22-25 Nov 2015

RVE-BASED MULTISCALE MODELING FOR THE NAVIER-STOKES EQUATIONS: LINKING CONTINUUM AND LATTICE-BOLTZMANN MODELS

Pablo J. Blanco[1,2,*]

Andrés R. Valdez[1,2]

Alejandro Clausse[3]

Raúl A. Feijóo[1,2]

[1] Laboratório Nacional de Computação Científica Av. Getúlio Vargas 333, 25651-075, Petrópolis, Rio de Janeiro, Brazil

[2] Instituto Nacional de Ciência e Tecnologia em Medicina Assistida por Computação Científica (INCT/MACC) Av. Getúlio Vargas 333, 25651-075, Petrópolis, Rio de Janeiro, Brazil

[3] Comisión Nacional de Energía Atómica, (CNEA-CONICET), Universidad Nacional del Centro, 7000 Tandil, Argentina

[*] pjblanco@lncc.br

Abstract. *This work addresses the multiscale modeling of fluid flow in highly involved media based on the concept of Representative Volume Element. Between scales we consider as basic principles for downscaling information the conservation of the velocity vector field and the conservation of the strain rate tensor field. In this context we formulate (i) the problem to be solved in the representative volume element (at fine scale), and (ii) the homogenization formulae for the force-like and the stress-like fields (at coarse scale) which stand for the procedure of upscaling data. Flow equations corresponding to simple fluids are considered at the coarse scale, and the classical Navier-Stokes equations are approximated in the fine scale by using the Lattice-Boltzmann method. Examples of application of flow in permeable media with small obstacles are presented to show the potentialities of the present approach.*

Keywords: *Complex fluids, Multiscale, Obstacles, Lattice-Boltzmann*

1 INTRODUCTION

Fluid flow simulations in complex media cover several fields of applications and lines of research. Specialized literature has been witness of a compelling need for improving predictive capabilities of models regarding the simulation of fluid flow under intricate conditions. For the context of the present work, complex conditions are those imposed by complex domains through which the fluid flows. Geometric features defined at several spatial lengths pose challenges for the theoretical analysis as well as for the numerical treatment of these problems. Porous media are the typical example for which continuum models have been modified from the Navier-Stokes equations to account for observable phenomena at a reasonable cost, disregarding thus the highly detailed flow complexity occurring at the level of pores. In such case it is evident the existence of a coarse scale conception (the porous media flow model) and fine scale flow properties determined by the geometric features of the pores.

The celebrated Darcy equation is the widely used approach to model fluid flow in porous media. Providing the Darcy equation with suitable constitutive equations (relating the velocity field to the pressure field at the coarse scale) yields a closed description of the flow at the coarse scale. However, phenomenological descriptions of these constitutive equations find strong limitations as the problem deviates from the original Darcy hypothesis, and approaches the flow regime described by the Navier-Stokes equations.

Multiscale modeling in fluid mechanics has been dominated by the asymptotic analysis technique (Allaire, 1991, 1992; Nguetseng and Signing, 2009; Griebel and Klitz, 2010; Brown et al., 2011; Icardi et al., 2014). The main hypothesis behind this approach is the separation of scales. The asymptotic approach is able to deliver the coarse scale equations once a fine scale phenomenon is postulated. Thus, from the Navier-Stokes equations it is possible to obtain the Darcy equation under proper hypotheses. However, no advances have been seen in trying to generalize this approach to deal with complex media, such as permeable media and flow regimes which depart from such standard hypotheses.

In turn, multiscale modeling in solid mechanics relying on the concept of representative volume element (RVE) is an extremely mature area of research. Within this framework, separation of scales is not longer a restriction, and a rich variety of complex physical phenomena can be retrieved from fine scale analysis. This approach has been completely overlooked in the field of fluid mechanics, short for the still largely phenomenological two-fluid model of two-phase flow. However, recent contributions have aproached the multiscale modeling in fluid mechanics using a similar concept of homogenization (Hou et al., 2013; Sandström and Larsson, 2013). Moreover, this is becoming increasingly important in bioengineering applications because of the intrinsic multiscale nature of physiological flows (Lei et al., 2013).

In the context of flow in porous and permeable media, the Lattice-Boltzmann (LB) model has been extensively and successfully applied. In such cases, the LB model is able to provide a phenomenological description at a certain scale (mesoscale) which represents some observable coarse scale physics. Nevertheless, no direct connection between the LB model and continuum equations have been established in the sense of homogenization in a RVE.

In the present work we address the multiscale modeling of fluid flow based on the concept of RVE. At the coarse scale we consider a quite standard flow model, while at the fine scale the model corresponds to the Navier-Stokes equations in domains containing obstacles. Considering a suitable downscaling strategy, and making use of adequate variational formulations we develop the problem to be solved at the fine scale (the RVE problem) as well as the homogenization rules for force- and stress-like entities which are required to close the problem at the coarse scale. That is, we proposed a strategy to compute a velocity field at a fine scale, from which proper homogenization formulae is applied such that relevant coarse scale quantities are retrieved.

This work is organized as follows. The coarse scale flow problem is presented in Section 2. The downscaling procedure to map coarse scale quantities into the fine scale is discussed in Section 3. The so-defined problem at the fine scale is formulated in Section 4. Homogenization rules to retrieve coarse scale quantities from the fine scale field are presented in Section 5. Section 6 describes the numerical tools to solve the problem at the fine scale, and some numerical results are reported in Section 7. Final remarks are outlined in Section 8.

2 COARSE SCALE FLOW MODELING

In the present work, we consider the following hypotheses for the flow problem at the coarse scale

H1) Two spatial scales are identified, namely a coarse and a fine scale.

H2) Fluid flow is stationary for both spatial scales.

H3) Fluid flow is described by a classical velocity field at both scales.

H4) Flow is incompressible at the fine scale.

H5) Flow is single phase and Newtonian at the fine scale.

H6) The fine scale contains rigid fixed obstacles through which the fluid flows.

Because of these hypotheses the flow at the coarse scale is also incompressible.

Let us formulate the incompressible flow problem at the coarse scale in a bounded domain $\Omega \in \mathbb{R}^n$, $n = 2, 3$, with boundary $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ (D: Dirichlet, N: Neumann) with outward unit normal $\mathbf{N}$. Given $\mathbf{C}$ and $\boldsymbol{\Sigma}$, a force-like and a stress-like object, respectively, the system is governed by the following set of differential equations

$$\begin{cases} \mathbf{C} - \mathrm{div}_\Omega\, \boldsymbol{\Sigma} + \nabla P = 0 & \text{in } \Omega, \\ \mathrm{div}_\Omega\, \mathbf{U} = 0 & \text{in } \Omega, \\ -P\mathbf{N} + \boldsymbol{\Sigma}^T\mathbf{N} = \mathbf{T} & \text{in } \partial\Omega_N, \\ \mathbf{U} = \overline{\mathbf{U}} & \text{in } \partial\Omega_D \end{cases} \tag{1}$$

where $\mathbf{U}$ is the fluid velocity field, P is the pressure field, ∇_Ω is the gradient operator with respect to coordinates $\mathbf{X} \in \Omega$, $\mathbf{T}$ and $\overline{\mathbf{U}}$ are known data.

For this problem to be well-posed it is necessary to specify

(i) a volumetric force $\mathbf{C}$;

(ii) a stress tensor $\boldsymbol{\Sigma}$.

In the classical single-scale Navier-Stokes setting, and denoting $\mathbf{G} = \nabla_\Omega \mathbf{U}$, these objects are

$$\mathbf{C}_{\mathrm{NS}} = \rho(\nabla_\Omega \mathbf{U})\mathbf{U} = \rho\mathbf{G}\mathbf{U}, \tag{2}$$

$$\boldsymbol{\Sigma}_{\mathrm{NS}} = 2\mu\nabla_\Omega^S \mathbf{U} = 2\mu\mathbf{G}^S. \tag{3}$$

where ρ and μ are the density and viscosity of the fluid, respectively, ∇_{Ω}^{S} is the symmetric gradient operator ($(\cdot)^S$ the symmetrization operation).

It is important to observe that $\mathbf{G}$ is a traceless tensor, i.e. $\mathrm{div}_{\Omega}\,\mathbf{U} = \mathrm{tr}\,\mathbf{G} = 0$, which implies that $\mathbf{G} = \mathbf{G}^D$, where $(\cdot)^D$ denotes the deviatoric component obtained as $(\cdot)^D = (\cdot) - \frac{1}{n}\,\mathrm{tr}(\cdot)$, with $n = 2, 3$.

Thus, the goal of the multiscale modeling approach to be developed in the forthcoming sections is to provide equation (1) with closure equations for the pair $(\mathbf{C}, \boldsymbol{\Sigma})$ as a function of the pair $(\mathbf{U}, \mathbf{G})$. Note that these equations in general will differ from equations (2) and (3), for they will convey the influence of the microstructures in the form of special forces and stresses. Specifically, the Lattice-Boltzmann method will be used to solve a flow problem at the fine scale from which these closure equations will be retrieved. The schematic multiscale procedure to be considered in this work is shown in Figure 1.

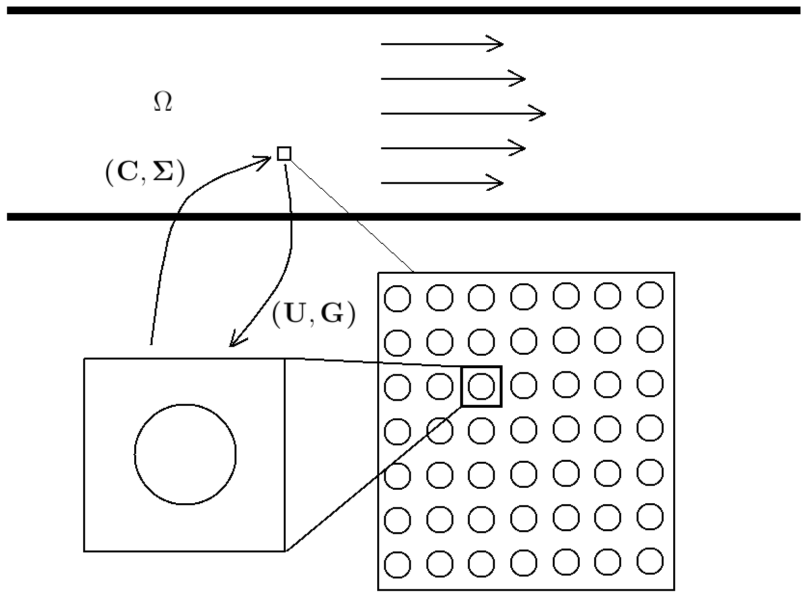

Figure 1: Multiscale modeling of the flow of a fluid using the concept of RVE.

3 DOWNSCALING PROCEDURE

For each point at the coarse scale we associate a fixed fluid Representative Volume Element (RVE, or simply cell) fixed in space and time, through which the fluid flows amid obstacles.

At the coarse scale the fluid velocity vector field is $\mathbf{U}$ and the velocity gradient is denoted by $\mathbf{G} = \nabla_{\Omega}\mathbf{U}$. These fields are defined in Ω, whose coordinates are $\mathbf{X}$. At the fine scale, the RVE domain is denoted by $\omega \subset \mathbb{R}^n$, with boundary $\partial\omega$ (outward unit normal $\mathbf{n}$). Coordinates in ω are denoted by $\mathbf{x}$. For simplicity it is assumed that $\int_{\omega} \mathbf{x}\, d\omega = 0$. In addition, we denote γ the boundaries of the obstacles in the fine scale which are internal in the RVE, and $\partial\omega$ the external boundary of the RVE whose outward unit normal is denoted by $\mathbf{n}$.

The velocity field is denoted by $\mathbf{u}$, and in the RVE domain ω, it is expanded as follows

$$\mathbf{u} = \mathbf{U} + \mathbf{G}\mathbf{x} + \tilde{\mathbf{u}}, \tag{4}$$

where, from the coarse scale we have $\mathbf{U} + \mathbf{G}\mathbf{x}$, and we consider an additional fluctuation field $\tilde{\mathbf{u}}$ at the fine scale. Besides, we have

$$\nabla_\omega \mathbf{u} = \mathbf{G} + \nabla_\omega \tilde{\mathbf{u}}, \tag{5}$$

where ∇_ω is the gradient operator with respect to coordinates $\mathbf{x} \in \omega$.

We consider that the following relations must be satisfied for the fields defined in different scales to be consistently coupled

$$\mathbf{U} = \frac{1}{|\omega|} \int_\omega \mathbf{u} \, d\omega, \tag{6}$$

$$\mathbf{G} = \frac{1}{|\omega|} \int_\omega \nabla_\omega \mathbf{u} \, d\omega. \tag{7}$$

These relations establish the criteria behind the downscaling of quantities defined at the coarse scale. Equivalently, integrating by parts, constraint (7) can be written as

$$\mathbf{G} = \frac{1}{|\omega|} \int_{\partial\omega} \mathbf{u} \otimes \mathbf{n} \, d\partial\omega. \tag{8}$$

4 FINE SCALE FLOW MODELING

The flow problem at the fine scale is ruled by the classical Navier-Stokes problem. Recall that we consider the flow to occur amid obstacles, for which we have the following no-slip condition

$$\mathbf{u} = 0 \qquad \text{on } \gamma. \tag{9}$$

In addition, we have to consider constraints (6) and (8). Thus, the problem is formulated as follows

$$\begin{cases} \rho(\nabla_\omega \mathbf{u})\mathbf{u} - \mu \Delta_\omega \mathbf{u} + \nabla_\omega p = \mathbf{b} & \text{in } \omega, \\ \operatorname{div}_\omega \mathbf{u} = 0 & \text{in } \omega, \\ (-p\mathbf{I} + 2\mu \nabla^S_\omega \mathbf{u})\mathbf{n} = \mathbf{t} & \text{on } \partial\omega, \\ (-p\mathbf{I} + 2\mu \nabla^S_\omega \mathbf{u})\mathbf{n} = \mathbf{r} & \text{on } \gamma. \end{cases} \tag{10}$$

where p is the pressure field at the fine scale, $\mathbf{b}$ is a force per unit volume which is such that it enforces the constraint (6), $\mathbf{t}$ is a force per unit surface which is such that it enforces the constraint (8) and $\mathbf{r}$ is also a force per unit surface that enforces the constraint (9).

A detailed derivation of the flow problem at the fine scale and the motivation and implications for constraints (6) and (7) can be found in Blanco et al. (2015).

5 UPSCALING PROCEDURE

Up to this point, we have presented

- the flow problem at the coarse scale given by the set of equations (1);

- the downscaling of quantities from the coarse scale as given by expressions (6) and (8);
- and the flow problem at the fine scale given by the set of equations (10).

Therefore, the issue which is still pending is the definition of the expressions for $\mathbf{C}$ and $\mathbf{\Sigma}$ which, respectively, play the role of a force and a stress tensor in (1), in compliance with the downscaling procedure defined above and the flow problem postulated at the fine scale. The definition of the pair $(\mathbf{C}, \mathbf{\Sigma})$ from variables defined in the RVE domain is called the upscaling procedure.

In (Blanco et al., 2015) a methodology based on variational principles allowed us to naturally derive the upscaling procedure such that we have a consistent physical coupling between scales in terms of energetic considerations involving virtual power at both scales.

Thus, the closed forms for $\mathbf{C}$ is given by the following homogenization equation

$$\mathbf{C} = \frac{1}{|\omega|}\left[\int_\omega \rho(\nabla_\omega \mathbf{u})\mathbf{u}\, d\omega - \int_\gamma \mathbf{r}\, d\gamma\right]. \tag{11}$$

while for $\mathbf{\Sigma}$ it is

$$\mathbf{\Sigma} = \frac{1}{|\omega|}\left[\int_\omega \left[\left[\rho(\nabla_\omega \mathbf{u})\mathbf{u}\right] \otimes \mathbf{x} + 2\mu \nabla_\omega^S \mathbf{u}\right] d\omega - \int_\gamma \mathbf{r} \otimes \mathbf{x}\, d\gamma\right]^D, \tag{12}$$

These two entities can be understood as composed by the classical Navier-Stokes terms corrected by higher order contributions derived from complex flow patterns at the fine scale, that is

$$\mathbf{C} = \mathbf{C}_{\mathrm{NS}} + \widetilde{\mathbf{C}}, \tag{13}$$

$$\mathbf{\Sigma} = \mathbf{\Sigma}_{\mathrm{NS}} + \widetilde{\mathbf{\Sigma}}. \tag{14}$$

where $\mathbf{C}_{\mathrm{NS}}$ and $\mathbf{\Sigma}_{\mathrm{NS}}$ are given by (2) and (3), respectively, and the fluctuations $\widetilde{\mathbf{C}}$ and $\widetilde{\mathbf{\Sigma}}$ exclusively depend on the velocity field and the forces over the obstacles at the fine scale.

6 NUMERICAL METHODS

The flow problem at the fine scale is solved using the Lattice-Boltzmann method. We consider for simplicity our problem in $\mathbb{R}^2$. We employ the Lattice-Boltzmann quasi incompressible scheme given by the D2Q9 cell as proposed by He and Luo (1997). Accordingly, the state of each grid point $\mathbf{x}$ at time t is given by nine scalars f_i associated with nine grid directions $\mathbf{e}_i$ (i: 1-4 Cartesian, 5-8 diagonal, and 0 stagnation). The corresponding governing equation for f_i is:

$$f_i(\mathbf{x} + \Delta x \mathbf{e}_i, t + \Delta t) = f_i(\mathbf{x}, t) + \frac{1}{\tau}\left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t)\right] + S_i(\mathbf{x}, t) \qquad i = 0, \ldots, 8 \tag{15}$$

where the equilibrium distribution f_i^{eq} is given by

$$f_i^{\mathrm{eq}} = w_i\left[\rho + \rho_0\left(3\frac{v\mathbf{e}_i \cdot \mathbf{u}}{v^2} + \frac{9}{2}\frac{(v\mathbf{e}_i \cdot \mathbf{u})^2}{v^4} - \frac{3}{2}\frac{\mathbf{u} \cdot \mathbf{u}}{v^2}\right)\right] \qquad i = 0, \ldots, 8 \tag{16}$$

S_i is an external source term, $v = \frac{\Delta x}{\Delta t}$, and ρ_0 is the average density and

$$w_0 = \frac{4}{9} \qquad w_{1-4} = \frac{1}{9} \qquad w_{5-8} = \frac{1}{36}. \tag{17}$$

This equilibrium distribution is specially suitable for problems in which it is crucial to maintain the divergence of the velocity field as low as possible.

As usual, density and velocity fields are computed as follows

$$\rho(\mathbf{x}, t) = \sum_{i=0}^{8} f_i(\mathbf{x}, t), \tag{18}$$

$$\mathbf{u}(\mathbf{x}, t) = \frac{v}{\rho_0} \sum_{i=0}^{8} f_i(\mathbf{x}, t)\mathbf{e}_i. \tag{19}$$

The fluid kinematic viscosity is then characterized through the relaxation parameter τ as follows

$$\nu = \frac{\mu}{\rho_0} = \frac{1}{3}\left(\tau - \frac{1}{2}\right)\frac{\Delta x^2}{\Delta t} \tag{20}$$

Differently from standart Lattice-Boltzmann schemes, in the present work, the flow problem at the fine scale requires the imposition of constraints (6), (8) and (9). As said before, these constraints are enforced by applying forces acting over the cells in correspondence with the following

$$\begin{aligned} \mathbf{b} &\rightarrow \text{ acting over } \omega, \\ \mathbf{t} &\rightarrow \text{ acting over } \partial\omega, \\ \mathbf{r} &\rightarrow \text{ acting over } \gamma, \end{aligned} \tag{21}$$

Observe that, according to the target constraint of each force, $\mathbf{b}$ is constant throughout the entire volume ω, the resultant of $\mathbf{t}$ should be null (more specifically it is constant over each side of the boundary $\partial\omega$) and $\mathbf{r}$ is a point-wise force defined at the bounday of the obstacles.

These forces are effectively applied through the following proportional-integral controller, described here for a generic force $\mathbf{f}$ as

$$\mathbf{f}(\mathbf{x}, t) = \alpha_{\mathbf{f}}(\mathbf{d} - h(\mathbf{u}(\mathbf{x}, t))) + \beta_{\mathbf{f}} \int_0^t (\mathbf{d} - h(\mathbf{u}(\mathbf{x}, \tau)))\, d\tau \tag{22}$$

where $\alpha_{\mathbf{f}}$ and $\beta_{\mathbf{f}}$ are appropriate control parameters, $h(\cdot)$ is a function of the velocity field that characterizes the constrain and $\mathbf{d}$ is the given datum.

For the forces specified in (21) we have the following controllers

$$
\begin{aligned}
\mathbf{b} &= \alpha_{\mathbf{b}}\big(|\omega|\mathbf{U} - \textstyle\int_\omega \mathbf{u}\, d\omega\big) + \beta_{\mathbf{b}} \int_0^t \big(|\omega|\mathbf{U} - \int_\omega \mathbf{u}\, d\omega\big)\, d\tau && \text{in } \omega, && (23)\\
t_x^{\mathrm{W}} &= \alpha_{\mathbf{t}}\big(|\omega|G_{xx} - \textstyle\int_{\partial\omega_{\mathrm{W}}} u_x\, d\partial\omega + \int_{\partial\omega_{\mathrm{E}}} u_x\, d\partial\omega\big) && && \\
&\quad + \beta_{\mathbf{t}} \int_0^t \big(|\omega|G_{xx} - \textstyle\int_{\partial\omega_{\mathrm{W}}} u_x\, d\partial\omega + \int_{\partial\omega_{\mathrm{E}}} u_x\, d\partial\omega\big)\, d\tau && \text{on } \partial\omega_{\mathrm{W}}, && (24)\\
t_x^{\mathrm{E}} &= -t_x^{\mathrm{W}} && \text{on } \partial\omega_{\mathrm{E}}, && (25)\\
t_y^{\mathrm{W}} &= \alpha_{\mathbf{t}}\big(|\omega|G_{yx} - \textstyle\int_{\partial\omega_{\mathrm{W}}} u_y\, d\partial\omega + \int_{\partial\omega_{\mathrm{E}}} u_y\, d\partial\omega\big) && && \\
&\quad + \beta_{\mathbf{t}} \int_0^t \big(|\omega|G_{yx} - \textstyle\int_{\partial\omega_{\mathrm{W}}} u_y\, d\partial\omega + \int_{\partial\omega_{\mathrm{E}}} u_y\, d\partial\omega\big)\, d\tau && \text{on } \partial\omega_{\mathrm{W}}, && (26)\\
t_y^{\mathrm{E}} &= -t_y^{\mathrm{W}} && \text{on } \partial\omega_{\mathrm{E}}, && (27)\\
t_y^{\mathrm{N}} &= \alpha_{\mathbf{t}}\big(|\omega|G_{yy} - \textstyle\int_{\partial\omega_{\mathrm{N}}} u_y\, d\partial\omega + \int_{\partial\omega_{\mathrm{S}}} u_y\, d\partial\omega\big) && && \\
&\quad + \beta_{\mathbf{t}} \int_0^t \big(|\omega|G_{yy} - \textstyle\int_{\partial\omega_{\mathrm{N}}} u_y\, d\partial\omega + \int_{\partial\omega_{\mathrm{S}}} u_y\, d\partial\omega\big)\, d\tau && \text{on } \partial\omega_{\mathrm{N}}, && (28)\\
t_y^{\mathrm{S}} &= -t_y^{\mathrm{N}} && \text{on } \partial\omega_{\mathrm{S}}, && (29)\\
t_x^{\mathrm{N}} &= \alpha_{\mathbf{t}}\big(|\omega|G_{xy} - \textstyle\int_{\partial\omega_{\mathrm{N}}} u_x\, d\partial\omega + \int_{\partial\omega_{\mathrm{S}}} u_x\, d\partial\omega\big) && && \\
&\quad + \beta_{\mathbf{t}} \int_0^t \big(|\omega|G_{xy} - \textstyle\int_{\partial\omega_{\mathrm{N}}} u_x\, d\partial\omega + \int_{\partial\omega_{\mathrm{S}}} u_x\, d\partial\omega\big)\, d\tau && \text{on } \partial\omega_{\mathrm{N}}, && (30)\\
t_x^{\mathrm{S}} &= -t_x^{\mathrm{N}} && \text{on } \partial\omega_{\mathrm{S}}, && (31)\\
\mathbf{r} &= \alpha_{\mathbf{r}}(-\mathbf{u}) + \beta_{\mathbf{r}} \int_0^t (-\mathbf{u})\, d\tau && \text{on } \gamma. && (32)
\end{aligned}
$$

where we have $\partial\omega = \partial\omega_{\mathrm{E}} \cup \partial\omega_{\mathrm{W}} \cup \partial\omega_{\mathrm{S}} \cup \partial\omega_{\mathrm{N}}$, as shown in Figure 2.

Control parameters are chosen such that the problem remains stable. The order of magnitude of the different parameters is reported in Table 1.

$\alpha_{\mathbf{b}}$	$\beta_{\mathbf{b}}$	$\alpha_{\mathbf{t}}$	$\beta_{\mathbf{t}}$	$\alpha_{\mathbf{r}}$	$\beta_{\mathbf{r}}$
$1 \cdot 10^{-3}$	$1 \cdot 10^{-4}$	$1 \cdot 10^{-3}$	$1 \cdot 10^{-4}$	$1 \cdot 10^{-6}$	$1 \cdot 10^{-8}$

Table 1: Recommended order of magnitude of controller parameters for the different force terms.

Any force is applied in the Lattice-Boltzmann equation by adding a consistent source term as in (Mohamad and Kuzmin, 2010)

$$S_i^{\mathbf{f}}(\mathbf{x}, t) = \frac{\Delta t}{3} w_i \mathbf{f}(\mathbf{x}, t) \cdot \mathbf{e}_i \qquad i = 0, \ldots, 8 \tag{33}$$

The flow problem at the fine scale takes place in a squared RVE as shown in Figure 2. For the Lattice-Boltzmann problem to be closed it is necessary to provide a complete set of boundary conditions. In the present work we extend the domain of the RVE making use of an artificial frame domain, denoted by $\tilde{\omega}$, surrounding the squared RVE. At the external boundary of this frame, called $\partial\tilde{\omega}$, we impose periodic boundary conditions for all functions f_i, $i = 0, \ldots, 8$.

The problem that will be addressed is a steady-state flow; therefore the time-dependent Lattice-Boltzmann problem is solved until the steady state is reached.

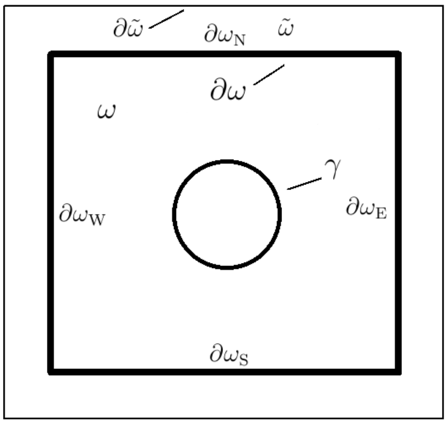

Figure 2: RVE domain with obstacle of circular shape and extension of the domain to impose periodic boundary conditions.

Notice that here we are making use of the Lattice-Boltzmann method as a numerical methodology to solve the system of equations given by (10). However, the present method is still valid for any flow problem defined at the fine scale, either given by a system of partial differential equations solved by the Lattice-Boltzmann method or given by a discrete dynamics addressed through the Lattice-Boltzmann method, but without no strict connection with a specific system of partial differential equations.

7 NUMERICAL RESULTS

To test the capabilities of the proposed multiscale method we consider the problem of the flow of a fluid in a channel with a buffer located at the mid part of the channel to divert flow as shown in Figure 3. Within the channel an array of obstacles with circular shape is introduced.

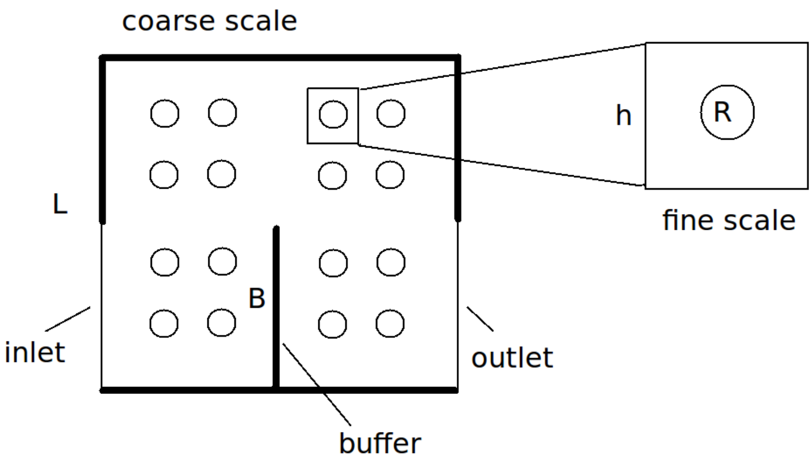

Figure 3: Flow in a channel with a buffer and obstacles.

Let us define the coarse scale flow problem. The channel has an inlet and an outlet. A pressure difference between inlet and outlet is imposed. The rest of the boundaries of the channel and at the buffer surface no-slip boundary conditions are considered (thick lines in

Figure 3. The geometry of the square is characterized by a side size L = 100, buffer size B = 50 and circular obstacles of radius R = 4. The size of inlet and outlet is also B. For such configuration, 16 squared cells were defined, each with size h = 20, which are to be regarded as RVEs.

To assess the capabilities of the present multiscale approach we firstly solve the flow problem at the coarse scale including all the geometric complexity in the problem. This simulation can be understood as a DNS (Direct Numerical Simulation) test, which is our gold standard. The numerical solution of the flow problem is obtained using the classical LBM with standard no-slip and pressure boundary conditions. Figure 4 shows the contour maps of the components of the velocity field (u_x top panel and u_y bottom panel) in the domain of the channel.

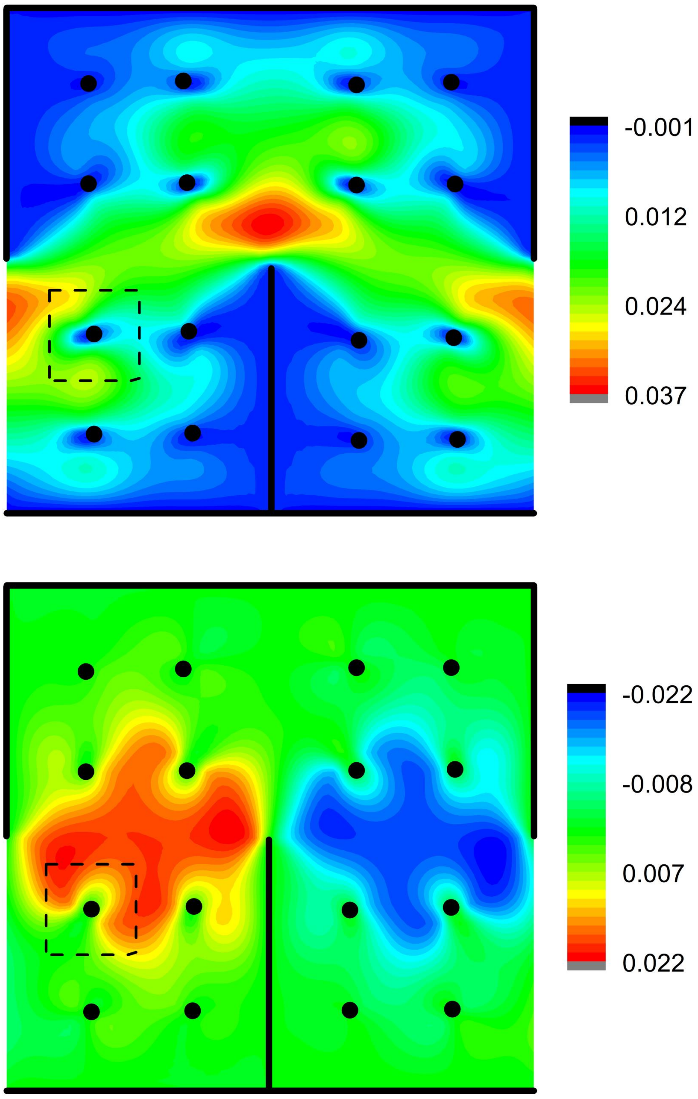

Figure 4: Flow field (u_x top, u_y bottom) in the channel obtained with direct numerical simulation.

Then, with the solution obtained from the DNS (flow featured in Figure 4) we compute in each one of the 16 cells the homogenization of the velocity vector field and of the gradient tensor field, denoted here by $\mathbf{U}_{\mathrm{DNS}}$ and $\mathbf{G}_{\mathrm{DNS}}$, respectively, and also of the force and stress fields, denoted here by $\mathbf{C}_{\mathrm{DNS}}$ and $\mathbf{\Sigma}_{\mathrm{DNS}}$, as expressed by (11) and (12), respectively. Note that each cell corresponds to a single flow condition given by the pair $(\mathbf{U}_{\mathrm{DNS}}, \mathbf{G}_{\mathrm{DNS}})$.

To perform the comparison between the multiscale approach (denoted by RVE) and the DNS we consider the 16 different flow conditions at the 16 RVEs which are given by $(\mathbf{U}_{\mathrm{DNS}}, \mathbf{G}_{\mathrm{DNS}})$ and solve the flow problem formulated by (10) in the RVE under these data, resulting in the corresponding homogenized quantities $\mathbf{C}_{\mathrm{RVE}}$ and $\mathbf{\Sigma}_{\mathrm{RVE}}$ according to expressions (11) and (12), respectively.

Figure 5 presents the correlation between the true values of the components (x and y) of the vector field $\mathbf{C}$ (which are given by the DNS test) and the values obtained from solving the problem at the RVE employing the downscaling and upscaling procedure proposed in this work. Clearly, the optimal situation occurs when the RVE problem is capable of exactly reproducing the linear function for all cells.

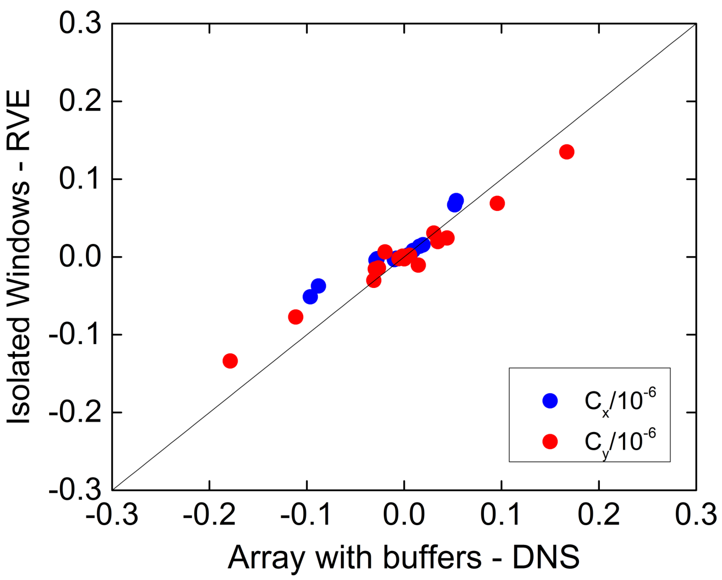

Figure 5: Correlation of components of the force vector field C between DNS **and** RVE**.**

Figure 6 presents the correlation between the values of the components (xx, yy, xy and yx) of the tensor field $\mathbf{\Sigma}$ given by the DNS test and the values obtained with the multiscale procedure at the RVE.

Remarkably, the correlation between the DNS case and the multiscale result referred to as RVE in the plots is strong, which provides convincing evidences of the predictive capabilities of the multiscale procedure. That is, the multiscale approach proposed in this work is capable of retrieving most of the physics present in the original single-scale problem. Indeed, to further verify and illustrate this statement consider the dashed window in the channel in Figure 4. That window corresponds to a specific RVE. Then, we compare the DNS velocity field in such window with velocity field obtained at the corresponding RVE when the coarse scale conditions at the window given by $(\mathbf{U}_{\mathrm{DNS}}, \mathbf{G}_{\mathrm{DNS}})$ are imposed. Figure 7 presents the components of the velocity field obtained from the DNS test and those from the RVE simulation for that specific window. It is notable that the flow patterns computed in the RVE are extremely close to the ones obtained from the DNS case, even in the present case in which separation of scales is not guaranteed.

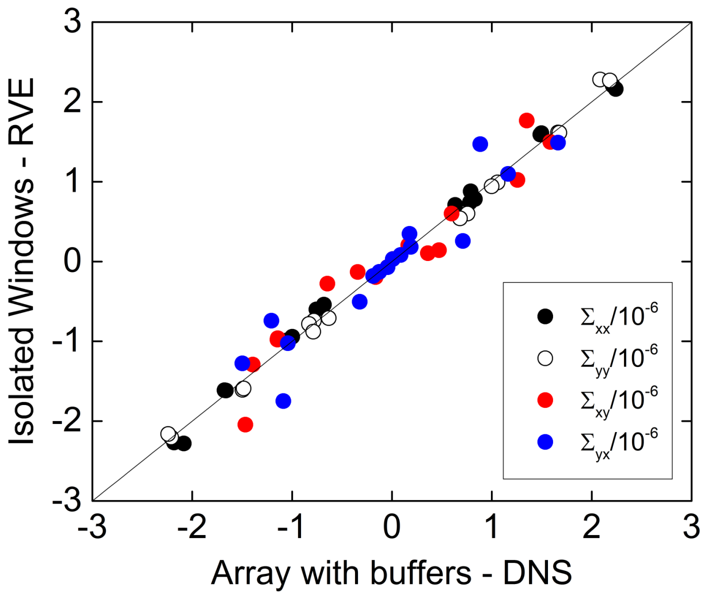

Figure 6: Correlation of components of the stress tensor field $\boldsymbol{\Sigma}$ between DNS and RVE.

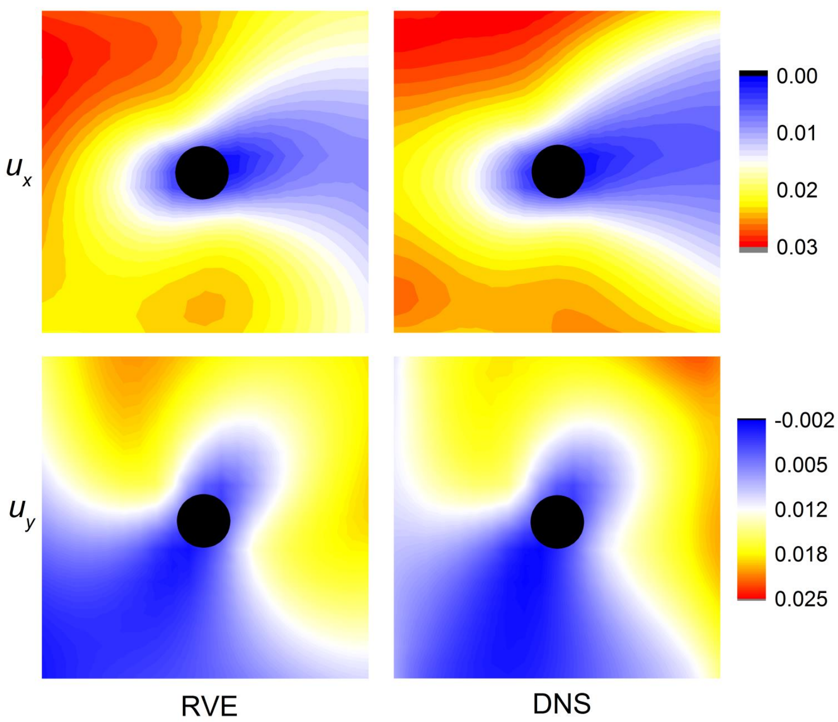

Figure 7: Components of the velocity field (u_x top, u_y bottom) from DNS and at the RVE.

8 FINAL REMARKS

In this work we have presented a methodology to couple two scales in fluid mechanics using the concept of Representative Volume Element. Proper homogenization rules were employed to retrieve from the fine scale force- and stress-like quantities to be used at the coarse scale. The fluid problem at the fine scale is ruled by the Navier-Stokes equations, for which the Lattice-Boltzmann method has been used as a numerical tool. Complex flow features beyond standard models can be obtained from the fine scale using a homogenization method based on variational principles. Moreover, it could be considered that the system at the fine scale is simply governed by the Lattice-Boltzmann equations without strict and necessary relation to the Navier-Stokes equations. This opens field to understand the way in which fine flow features as predicted by the Lattice-Boltzmann scheme can impact continuum models of fluid mechanics.

ACKNOWLEDGEMENTS

This work was partially supported by the Brazilian agencies CNPq and FAPERJ. The support of these agencies is gratefully acknowledged.

REFERENCES

Allaire, G., 1991. Homogenization and two-scale convergence. *Arch. Rational Mech. Anal.*, vol. 113, pp. 261–298.

Allaire, G., 1992. Homogenization and two-scale convergence. *SIAM J. Math. Anal.*, vol. 23, pp. 1482–1518.

Blanco, P.J., Sánchez, P.J., de Souza Neto, E.A., & Feijóo, R.A., 2015. Variational foundations and generalized unified theory of RVE-based multiscale models. *Archives of Computational Methods in Engineering*, In Press:doi: 10.1007/s11831–014–9137–5.

Brown, D.L., Popov, P., & Efendiev, Y., 2011. On homogenization of stokes flow in slowly varying media with applications to fluidstructure interaction. *Int. J. Geomath.*, vol. 2, pp. 281–305.

Griebel, M., & Klitz, M., 2010. Homogenization and numerical simulation of flow in geometries with textile microstructures. *Multiscale Model. Simul.*, vol. 8, pp. 1439–1460.

He, X., & Luo, L.S., 1997. Lattice-Boltzmann model for the incompressible navierstokes equation. *J. Stat. Phys.*, vol. 88, pp. 927–944.

Hou, T.Y., Hua, X., & Hussain, F., 2013. Multiscale modeling of incompressible turbulent flows. *J. Comput. Phys.*, vol. 232, pp. 383–396.

Icardi, M., Boccardo, G., Marchisio, D.L., Tosco, T., & Sethi, R., 2014. Pore-scale simulation of fluid flow and solute dispersion in three-dimensional porous media. *Physical Review E*, vol. 90, pp. 013032.

Lei, H., Fedosov, D.A., Caswell, B., & Karniadakis ,G.E., 2013. Blood flow in small tubes: quantifying the transition to the non-continuum regime. *J. Fluid Mech.*, vol. 722, pp. 214–239.

Mohamad, A.A., & Kuzmin, A., 2010. A critical evaluation of force term in lattice boltzmann method, natural convection problem. *International Journal of Heat and Mass Transfer*, vol. 53, pp. 990–996.

Nguetseng, G., & Signing, L., 2009. Sigma-convergence of stationary navier-stokes type equations. *Electronic Journal of Differential Equations*, vol. 74, pp. 1–18.

Sandström, C., & Larsson, F., 2013. Variationally consistent homogenization of stokes flowin porous media. *Journal for Multiscale Computational Engineering*, vol. 11, pp. 117–138.