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Multiscale modeling of blood flow: Coupling finite elements with smoothed dissipative particle dynamics

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Abstract

A variational multi scale approach to model blood flow through arteries is proposed. A finite element discretization to represent the coarse scales (macro size), is coupled to smoothed dissipative particle dynamics that captures the fine scale features (micro scale). Blood is assumed to be incompressible, and flow is described through the Navier Stokes equation. The proposed coupling is tested with two benchmark problems, in fully coupled systems. Further refinements of the model can be incorporated in order to explicitly include blood constituents and non-Newtonian behavior. The suggested algorithm can be used with any particle-based method able to solve the Navier-Stokes equation.

Keywords: Blood flow; Variational Multiscale; Smoothed dissipative particle dynamics.

1. Introduction

Cardiovascular diseases are one of the deadliest diseases in the world, killing more people than cancer every year [1]. Thus, the study of blood flow through the cardiovascular system emerges as an active research field nowadays. Improving our understanding of the physical phenomena occurring at all scales (from arteries to capillaries), as well as their link to disease, could have a positive impact on public health.

Different approaches have been taken to model cardiovascular systems, ranging from merely homogeneous (or heterogeneous) continuum description [2], [3], to micro scale particle descriptions [4], [5]. Some of these methodologies have attempted to model blood constituents explicitly, such as red blood cells [6], [7], and, platelets in regions on the scale of micrometers, in order to recover micro-scale interactions. Alternatively, homogeneous descriptions of the blood have been done to reproduce global hydrodynamic effects [8]. Hybrid methods that allow to capture both local and global effects are still under development due to the complexity of the cardiovascular system [9], [10], [11].

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Thrombus formation in large arteries can be described roughly as the coupled interactions at two different scales [12]: local flows involving aggregation-adhesion of blood constituents and global hemodynamics. In general, modelling of thrombus development with traditional description of continuum methods is approximate for bulk hemodynamics rather than local interactions.

The main goal in this work is to model hemodynamics in a simplified cardio vascular setting, using a representation that can capture both global and local effects. Enrichments may allow for clot formation modeling close to arterial walls. When the local effects occur at scales in the order of micrometers, the system is governed by fluctuating hydrodynamics equations [13]. These equations introduce the thermal and mechanical fluctuations responsible for the randomness of the Brownian motion. As the length scale of the system increases, these fluctuating hydrodynamics converge to the well known Navier-Stokes equation [14].

In order to couple micro and macro scales we use the variational multi scale (VMS) method [15], [16]. The VMS framework has been used in systems where additional physical features were included to enhance the physical representation, while improving the discrete stability. Relevant examples include the modelling of turbulence [17], [18], and porous media [19]. In the VMS context the fine scale solution is driven by the residual of the coarse scales. The solution of the VMS problem requires fine scale solution to be expressed as a projection of the coarse level.

Previous work coupling or improving the continuum models with particles descriptions can be found in the literature [20, 21, 22, 23], but none of those used the VMS approach.

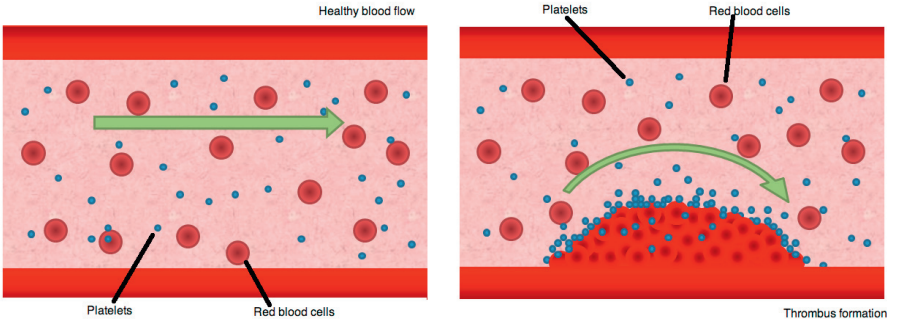

Fig. 1. Schematic representation of blood flow, where macro and meso-scale phenomena are coupled due to the presence of multiple constituents. The formed thrombus, originated at the fine scale, induces a posterior alteration in the hemodynamics at the macro scale.

2. Hemodynamic modeling

In this context, the dependent variables chosen to be studied are blood velocity and pressure. Additional information, such as transport properties of the blood fluid, are considered as input data [24] in the proposed model.

Due to the inherent high complexity in the cardiovascular systems, where multiple space-time scales and flow regimes are relevant, a set of initial assumptions is made: *i*) Newtonian fluid, *ii*) incompressible flow, *iii*) non-slip boundary condition at macro scale, *iv*) inertial effects presents, *v*) isothermal flow (macroscopically), but thermally fluctuating at meso-scale level, *vi*) Homogeneous flow. These assumptions can be eventually relaxed in the refinement process of the model. In our modeling description, we detail all the assumptions introduced. For the sake of simplicity, assumption (*i*) is stated, however, a rigorous model requires to consider the blood as a shear thinning like-fluid, due to the blood constituents. Newtonian assumption is in general suitable at high shear rates [24]. In future work including blood constituents, this assumption will no longer be adopted.

2.1. Navier-Stokes

We start out by writing the balance equations for mass and linear momentum, typically known as the Navier-Stokes equations, based on assumptions *i* through *vi*. Angular momentum and energy balances, as well as the

entropy inequality in the present model are satisfied by construction, and thus not evaluated.

The mass balance can be defined as:

$$\nabla \cdot \mathbf{v} = 0 \tag{1}$$

Assuming an arbitrary domain Ω, the momentum balance is given by:

$$\mathbf{v}_{,t} + \nabla \cdot (\mathbf{v} \otimes \mathbf{v}) + \nabla p - \nabla \cdot (2\frac{\mu}{\rho}\nabla^s \mathbf{v}) = f \quad in \quad \Omega\times]0, T[\tag{2}$$

where $\mathbf{v}$, p, ρ, μ and f are the fluid velocity, pressure, density, viscosity and external forces respectively.

The proposed hemodynamic describes in a simplified manner the whole fluid using Navier-Stokes equations. However, we aim to have a model that can capture the bulk behavior, including the surface contact, and, eventually thermal fluctuations at the mesoscale. This is why we focus on a meso-scale model, that can enrich the macro-scale description.

2.2. Variational Multiscale

In order to introduce the VMS approach we formally define a domain Ω, such that $\Omega \subset \mathbb{R}^d$, where $d \geq 1$ is the number of space dimensions, with a boundary Γ. The boundary-value problem is defined as:

Find $u : \Omega \to \mathbb{R}$ such that:

$$\mathcal{L}u = f \quad \text{in} \quad \Omega \tag{3}$$

$$u = g \quad \text{on} \quad \Gamma \tag{4}$$

where $f : \Omega \to \mathbb{R}$ and $g : \Gamma \to \mathbb{R}$ are given functions, and $\mathcal{L}$ is a second-order operator.

Let $S \subset H^1(\Omega)$ be the *trial solution space* and $V \subset H^1(\Omega)$ denote the *weighting function space*, where $H^1(\Omega)$ is the Sobolev space of square-integrable functions with square-integrable derivatives. We assume that S and V possess the following properties: $u = g$ on $\Gamma \; \forall \; u \in S$, and $w = 0$ on $\Gamma \; \forall \; w \in V$

The variational form of the current boundary-value problem can be written as:

Find $u \in S$ such that $\forall w \in V$

$$a(w, u) = (w, f) \tag{5}$$

Now, based on the VMS formulation [15], an additional assumption is included:

viii The solution of the different fields can be decomposed as a summation of multi-scale contributions.

Considering this, the problem can be stated as:

$$u = \bar{u} + u' \tag{6}$$

$$w = \bar{w} + w' \tag{7}$$

where $\bar{u}$ represents *coarse scales* and u' represents *fine scales* (see Fig. 2). This interpretation assumes that the coarse scale accounts for the smooth (and macro scale) behavior of the system, while the fine scale considers the highly oscillatory (and micro scale) part.

We use the following domain decomposition:

$S = \bar{S} \bigoplus S'$

$V = \bar{V} \bigoplus V'$

where $\bar{}$ and $'$ represent the coarse and fine scales, respectively. Following [15], some extra assumptions are made:

ix $\bar{u} = g$ on $\Gamma \; \forall \; \bar{u} \in \bar{S}$, $u' = 0$ on $\Gamma \; \forall \; u' \in S'$, $\bar{w} = 0$ on $\Gamma \; \forall \; \bar{w} \in \bar{V}$, and $w' = 0$ on $\Gamma \; \forall \; w' \in V'$

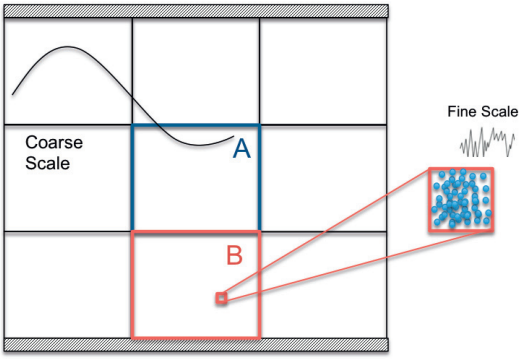

Fig. 2. Coarse and fine scale components.

By substituting equations (6) and (7) in (5) we get:

$$a(\bar{w}+w',\bar{u}+u') = (\bar{w}+w',f) \;\; \forall \bar{w} \in \bar{V}, \;\; \forall w' \in V' \tag{8}$$

Then, if $\bar{w}$ and w' are linearly independent, we have:

$$a(\bar{w},\bar{u}) + a(\bar{w},u') = (\bar{w},f) \;\; \forall \bar{w} \in \bar{V} \tag{9}$$

$$a(w',\bar{u}) + a(w',u') = (w',f) \;\; \forall w' \in V' \tag{10}$$

leading to:

$$a(\bar{w},\bar{u}) + (\mathcal{L}^*\bar{w},u') = (\bar{w},f) \;\; \textit{coarse scale problem} \tag{11}$$

$$a(w',\mathcal{L}\bar{u}) + (w',\mathcal{L}u') = (w',f) \;\; \textit{fine scale problem} \tag{12}$$

where $\mathcal{L}^*(\cdot)$ is the adjoin operator. Equation (12) is usually expressed as:

$$\Pi'\mathcal{L}u' = -\Pi'(\mathcal{L}\bar{u} - f) \;\; in\ \Omega \tag{13}$$

$$u' = 0 \;\; on\ \Gamma \tag{14}$$

The above equations illustrate that the fine scale problem is basically driven by the residual of the coarse scales, which can be seen as a new boundary value problem with an additional force term acting over the system. Following the VMS approach previously derived, now it is possible to write the weak formulation for the flow problem

$w = (\mathbf{w}, \mathbf{q})$

$$\int_\Omega \mathbf{w}[\mathbf{v}_{rt} + \nabla\cdot[(\mathbf{v}\otimes\mathbf{v}) + p\mathbf{I} - 2\nu\nabla^s\mathbf{v}] - \mathbf{f}] + \int_\Omega q\nabla\cdot\mathbf{v} = 0 \tag{15}$$

$$p = \bar{p} + p' \tag{16}$$

$$\mathbf{v} = \bar{\mathbf{v}} + \mathbf{v}' \tag{17}$$

Substituting (16) and (17) in (15), we have for the coarse scale that:

$$\begin{aligned} a(\bar{\mathbf{w}},\bar{\mathbf{v}}+\mathbf{v}') = {} & \int_\Omega \nabla\bar{\mathbf{w}}\cdot(2\mu\nabla\bar{\mathbf{v}} - \bar{\mathbf{v}}\otimes\bar{\mathbf{v}}) + \int_\Omega \nabla\bar{\mathbf{w}}\cdot(2\mu\nabla\mathbf{v}' - \mathbf{v}'\otimes\mathbf{v}') - \int_\Omega \nabla\bar{\mathbf{w}} \\ & \cdot(\bar{\mathbf{v}}\otimes\mathbf{v}' + \mathbf{v}'\otimes\bar{\mathbf{v}}) - \int_\Omega \nabla\cdot\bar{\mathbf{w}}(\bar{p}+p') + \int_\Omega \bar{q}(\nabla\bar{\mathbf{v}} + \nabla\mathbf{v}') \end{aligned} \tag{18}$$

$$L(\bar{\mathbf{w}}) = \int_{\Omega} \mathbf{w} \cdot ((\bar{\mathbf{v}}_{,t} + \mathbf{v}'_{,t}) - \mathbf{f}) \tag{19}$$

Equation (18) corresponds to the coarse scale problem, but is not the same as (11), due to the presence of cross terms: $(\bar{\mathbf{v}} \otimes \mathbf{v}' + \mathbf{v}' \otimes \bar{\mathbf{v}})$. In the proposed coupling procedure, equation (18) is discretized by finite element method, that can be found elsewhere [25]. On the other hand, although an equivalent expression of (18) can be formulated for the fine scale weak form, a particle-based discretization is proposed instead.

3. Fine-scale model: Smoothed dissipative particle dynamics

As is stated before in the VMS problem, it is necessary to define a fine scale formulation that can be used in equation (18); the aim is to get the fine scale solution of the system by a relatively new particle method, smoothed dissipative particle dynamics (SDPD) [26].

SDPD is a method that combines features of the well known smooth particle hydrodynamics (SPH) [27], and dissipative particle dynamics (DPD) [28]. This combination leads to a particle discretization of the Navier-Stokes equation, with the capability to consistently reproduce thermal fluctuation at the mesoscopic level [29]. In the case of blood flow, it is known that some of its main components, like red blood cells and platelets, are actually influenced by thermal fluctuations [30]. This kind of fluctuation must eventually be considered when local interactions at the level of wall interfaces are studied; thus, it is necessary to have a model capable of capturing meso-scales features.

3.1. SDPD model

In the framework of particle-based methods, an arbitrary function $f(\mathbf{x})$ can be represented by means of an integral interpolant in terms of a kernel function $W(\mathbf{x}, h)$ [31], such that:

$$\langle f(\mathbf{x}) \rangle = \int_{\Omega} f(\mathbf{x}')W(\mathbf{x} - \mathbf{x}', h)d\mathbf{x}' \tag{20}$$

The interpolant reproduces $f(\mathbf{x})$ exactly if the kernel is a delta function. In practical applications, the kernels are functions that are normalized to one in order to interpolate constants, and tend to delta functions as the support h goes to zero. In order to discretize any partial differential equation by a particle description, it is common to define an adequate kernel function $W(r)$ over which any property can be evaluated at the position of the particle, as a local average within some support h. For each particle we can define a mass m_p , a number of particle density $d_i = \sum_j W(\|\mathbf{r} - \mathbf{r}_j\|)$, and the volume of a particle $V_i = \frac{1}{d_i}$. The previous statement only satisfies $\sum V_i = V_{total}$ when the number of particles N tends to infinity. However, it can be assumed that above certain threshold $\sum V_i \approx V_{total}$. This threshold or minimum number of particles required can be easily fixed by choosing a tolerance value t_{vol} such that:

$$\frac{\sum V_i}{V_{total}} \leq t_{vol} \tag{21}$$

Based on this kernel function, any property $A(\mathbf{r})$ can be expressed as:

$$A(\mathbf{r}) = \frac{\sum_j W(|\mathbf{r} - \mathbf{r}_j|)A(\mathbf{r}_j)}{\sum W(|\mathbf{r} - \mathbf{r}_j|)} \tag{22}$$

In addition, in order to represent a partial differential equation, it is useful to approximate any derivative of the property, by taking the derivative of the kernel function $W(r)$. Lets define the gradient of W as:

$$\nabla W(r) = -F(r)\mathbf{r} \tag{23}$$

A common selection for this kernel function is the Lucy equation, widely used in SPH [26]:

$$W(r) = \frac{105}{16\pi h^2}(1 + 3\frac{r}{h})(1 - \frac{1}{h})^3 \tag{24}$$

where h is the support domain such that $h << L$, being L the domain length. With the selected kernel function, $F(r)$ can be written as:

$$F(r) = \frac{315}{4\pi h^5}(1 - r/h)^2 \tag{25}$$

Although, the SDPD discretization for the Navier-Stokes equation proposed by Espanol and Ravenga (2003) [26] is suitable for compressible flow, it is possible to take an approach frequently used with the lattice Boltzmann or with SPH [32], and consider the system as a weakly-compressible flow. The system is eventually compatible with the incompressibility assumption, if the time step size and the Mach number used are small enough [33]. The Navier-Stokes equation for the weakly-compressible system can be written in the SDPD form as:

$$m\frac{d}{dt}\mathbf{v}_i = \sum_j (\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2})F_{ij}\mathbf{r}_{ij} - (2\mu)\sum_j \frac{F_{ij}\mathbf{v}_{ij}}{d_i d_j} \tag{26}$$

where μ is the fluid viscosity, P is the pressure of the system and can be expressed as $P_i = P_i(d_i)$, where $P_i(d_i)$ is a regular equation of state. Here we choose a Tait's equation[34], with the form:

$$P = \frac{c_0^2\rho_0}{7}\left[\left(\frac{\rho}{\rho_0}\right)^7 - 1\right] \tag{27}$$

where c_0 is the artificial speed of sound for the fluid, and ρ_0 is a reference density. As one of the initial assumptions of the present model is the incompressibility of the flow, the value of a should be selected in order to get small Mach number ($Ma \leq 0.01$).

The presented SDPD discretization can be found in the paper of Espanol and Ravenga, the discretization for the second derivatives has a solid interpretation, and the general model for SDPD can be generalized with thermal fluctuations. It is the aim of the model proposed in this paper, that the thermal fluctuation be consistently included in a more refined model in a straightforward manner. The development of a coupling procedure between finite elements and SDPD has this capability by construction.

3.2. Fine Scale boundary condition

Since the cardiovascular systems of interest go roughly from sizes of the order of capillaries to the size of arteries, it is assumed for convenience that each finite element of the coarse scale constitutes a SDPD simulation box. Due to the scaling of thermal fluctuations [29], this assumption may take out the meso-scale features if this model is extended to larger domains. In that case mathematical homogenization procedures may be implemented, where each SDPD simulation can be used as a cell problem.

The proposed scale decomposition assumes that the fine scale feels or is driven by the residual of the coarse scale, with the fine scale not contributing anything beyond the boundaries of the elements. This assumption although strong, allows us to define the boundary for the particle fine scale domain, by setting walls of zero velocity particles at the edges of the box, interacting smoothly with the rest of fluid particles.

The boundary condition (BC) proposed, is neither non-slip nor slip condition in a rigorous sense, due to the smoothed kernel used in the interaction with the frozen wall.

4. Coupling algorithm

For the coupling procedure, an additional assumption can be included, making the variables independent of time at the coarse scale:

x Due to the separation in time scales between the fine and the coarse scale, the coarse scale is assumed to be in steady state, while the fine scale is fluctuating at high frequencies, and can be modeled as a transient system, tending to the equilibrium at time t_{eq}, such that: $\Delta t_{fine} << t_{eq} << \Delta t_{coarse}$

The proposed algorithm for coupling finite elements with smoothed dissipative particle dynamics is:

1. Solve

$$\int_\Omega \nabla\bar{\mathbf{w}} \cdot (2\mu\nabla\bar{\mathbf{v}} - \bar{\mathbf{v}} \otimes \bar{\mathbf{v}}) + \int_\Omega \nabla\bar{\mathbf{w}} \cdot (2\mu\nabla\mathbf{v}' - \mathbf{v}' \otimes \mathbf{v}') - \int_\Omega \nabla\bar{\mathbf{w}} \cdot (\bar{\mathbf{v}} \otimes \mathbf{v}' + \mathbf{v}' \otimes \bar{\mathbf{v}}) - \int_\Omega \nabla \cdot \bar{\mathbf{w}}(\bar{p} + p') + \int_\Omega \bar{q}(\nabla\bar{\mathbf{v}} + \nabla\mathbf{v}') = 0 \tag{28}$$

   where: $v' = 0, \quad p' = 0.$

2. In the elements where the fine scale is active, evaluate its residual using the current velocity and pressure fields. Run fine scale particle boxes with their respective elemental residual acting as a external force on the fine scale
3. Solve:

$$m\frac{d}{dt}\mathbf{v}_i = \sum_j (\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}) F_{ij}\mathbf{r}_{ij} - (2\mu)\sum_j \frac{F_{ij}\mathbf{v}_{ij}}{d_i d_j} - R_i \tag{29}$$

   where *Ri* is the residual of the coarse scale evaluated at the particle i as:

$$R_i = \frac{\sum_j W(|\mathbf{r}_i - \mathbf{r}_j|)R_j}{\sum_j W(|\mathbf{r}_i - \mathbf{r}_j|)} \tag{30}$$

4. Increase Δt_{fine} if:

$$\frac{\Delta v(\mathbf{r})}{v(\mathbf{r})} \geq \delta_{fine} \tag{31}$$

   where δ_{fine} is a tolerance value, $v(\mathbf{r})$ is the velocity at any arbitrary point $\mathbf{r}$, evaluated with the equation (30) and $\Delta v(\mathbf{r})$ is the difference of the velocity between the current and the previous time step.
5. Interpolate v' and p' over the Gauss points of the element, equation (30)
6. Repeat from step 1 with the new v' and p', until coarse scale convergence is reached, when:

$$R_i \leq \delta_{coarse} \tag{32}$$

   where δ_{coarse} is a tolerance value and R_i is the residual of the coarse scale elements

5. Simulations

To test the proposed coupling algorithm, driven cavity and 2D Poiseuille flow are studied, following the coupling algorithm proposed in the previous section. An initial set of simulations were carried out where the whole domain includes both coarse and fine scales. This scheme allows to study a fully two-way coupled system.

5.1. Simulation details

Coarse scales were discretized using Taylor-Hood finite elements (quadratic and cubic polynomials for pressure and velocity spaces respectively). $Re = 10^1$ to $Re = 10^3$ were evaluated in square domains of $(1cm)^2$, in meshes of sizes 8^2, 16^2, 32^2, 64^2 and 128^2. Fully coupled simulations used finite elements with particles resolution ranging from 500 to 4000 sdpd particles in the whole domain.
Parameters for fine scales were adopted to satisfy weakly incompressible blood flow (density fluctuations, $\delta\rho_i < 1\%$), and the maximum time step limited to Courant-Friedrichs-Lewy conditions [35]. The set up for sdpd simulations was: fluid kinematic viscosity $\mu = 3\text{x}10^{-3} Pa \cdot s$ [24], density $\rho = 1060 kg/m^3$, $\delta t = 5\text{x}10^{-6} s$, and artificial speed of sound $c = 0.1 m/s$, leading in all the simulations to Mach numbers of $Ma \approx 0.1$. The support for the kernel function was $h = 3\text{x}10^{-5} m$, and the particle mass ranged from $m_p = 2\text{x}10^{-4} kg$ to $2\text{x}10^{-5} kg$, depending on the number of particles in the system. The implementation of the zero velocity walls, was done by setting 4 additional layers of frozen particles at each side of the box.

5.2. Results

Mesh size smaller than 32^2, evidenced a poor resolution for the coarse-scale solution in the benchmark problem evaluated. In addition, when a small number of elements was used, the fine-scale was not able to countervail the lack in accuracy. The later is expected since the magnitude of the residual was similar for the different sizes.

In general, the fine-scale velocity profiles reached equilibrium around $0.1s$ (10^5 time steps), however, it was evident the need to use smaller time steps in order to ensure the simulation stability, as the coarse scale residual increase when Re does so.

The results obtained, showed that the coupling of sdpd fine scales did not generate instabilities in the global solution in any of the simulated systems. Furthermore, the resolved coarse scales are preserved (figure 3), while the fine scales are completely driven by the coarse scale residual. Figure (4) illustrates the reproduced coarse scale velocity, and the induced velocity profile in fine scale, leading to vortex formation. In Poiseuille flow simulations, counterflow close to the walls in fine scale level occurred at $Re = 1000$.

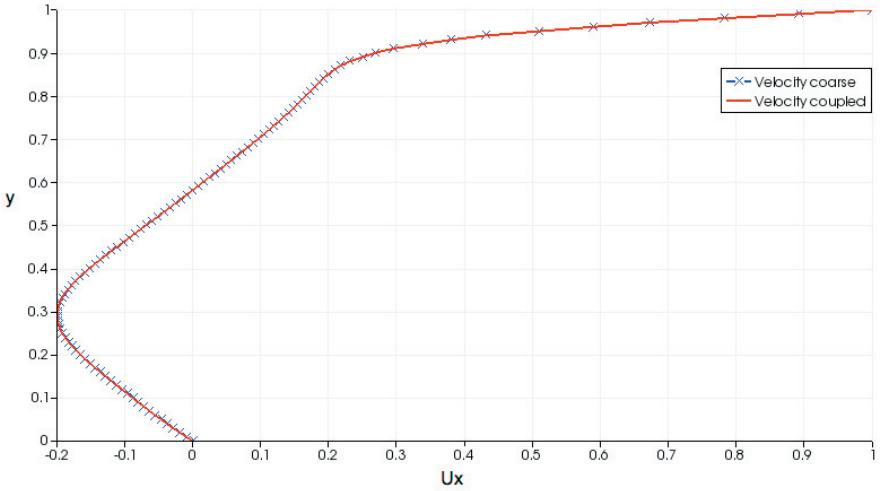

Fig. 3. Horizontal coarse-scale fluid velocity along the vertical center line for $Re = 10^3$. For the sake of comparison, the velocity profiles before (coarse) and after (coupled) fine scale coupling are presented.

The implemented procedure, although fully coupled, is behaving as one-way coupling. Only the fines scales are modified by the coarse level, while the macro-scale is not affected significantly. Nevertheless, in the limit where the fine scales get coarser (the mass of the particles increases), the trivial solution is recovered and the fine scale is no longer affected. It is worth mentioning that the inclusion of the fines scales showed a small decrease of the global error in the coarse scale. Further error analysis will be addressed in future work.

6. Conclusions

The proposed model allows a consistent coupling of particle-based methods such as SDPD with the continuum finite element method, that permits one to include relevant features of mesoscale. In the scope of the simulations setup used, the method behaves as a one-way coupling. In order to get a better description of blood flow, the current model requires improvements by considering non-newtonian fluid, explicit modeling of blood constituents

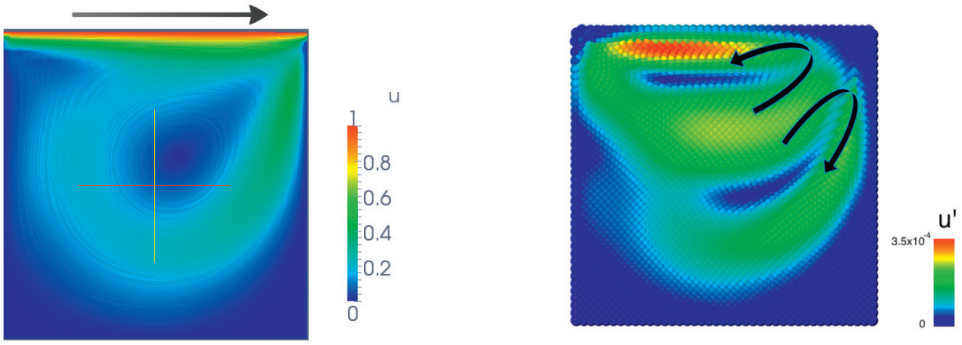

Fig. 4. Coarse (left) and fine (right) velocity profiles. SDPD fine scales are driven by the residual coarse scale. The current influence of the residual as external force, induces different vortex patterns in the simulation domain. The arrows indicate the flow direction.

and pulsatile flow; these aspects will be addressed in future work. One of the most important drawbacks in the stability of this model is the use of the weakly-compressible form of the SDPD model, penalizing the permissible time step. To avoid possible fine scale instabilities, it is necessary to include a fully incompressible particle description. The proposed coupling method is suitable for any particle-based method that can discretize a Navier-Stokes equation.

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