Efficient Implementation for Particle Tracing in Computational Hemodynamics

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Resumo. *Massless particle tracing is an important step towards acquiring a better insight of the complex phenomena that take place in the major vessels of the cardiovascular system. This makes possible to analyze hemodynamics factors that are believed to play a main role in the onset and progress of cardiovascular diseases such as long residence times, stagnation and/or high recirculation regions, among others. In addition, in this class of problems, numerical simulations provide large data sets, which must be processed in order to calculate the particle pathlines. Thus, the use of efficient computational implementations to deal with the tracking of particles in the blood flow is thus compulsory. In this work a series of tools devised to compute in an efficient manner these pathlines is presented. Emphasis is also given to the computation of pathlines corresponding to particles which remain in the vessel under analysis more than one cardiac cycle. This is accomplished by making use of a hypothesis of periodic blood flow.*

Keywords: *Particle Tracing, Fluid Hemodynamics*

1. Introduction

During the last years, a series of advances in terms of computational modeling and numerical simulation came into scene to provide a complementary framework for the analysis of the onset and progress of cardiovascular diseases. Preliminary results show that these tools are capable of giving an accurate insight in some surgical procedures as well as for medical training (Grinberg et al., 2009; Migliavacca et al., 2006). Nowadays, it is widely accepted that the evolution of some cardiovascular diseases, such as artery occlusion, arteriosclerosis and aneurysm growth depends upon hemodynamics factors related to the main phenomena taking place in the blood flow and in the arterial wall (A.M. Malek et al., 1999).

The HeMoLab system (Larrabide and Feijóo, 2006) was developed with the purpose of gathering in a single environment most of the computational tools needed for the numerical simulation of the cardiovascular system. Basically, HeMoLab is an integrated environment built on top of Paraview which allows: (i) the creation of patient-specific geometries of arterial vessels obtained from medical images, (ii) the coupling of such 3D geometries with a 1D model of the arterial tree, (iii) the numerical simulation of such model and (iv) the visualization of the results for analysis. Concerning the post-processing stage (step (iv)), the development of visualization techniques specifically devised for dealing with pulsatile fluid flows is essential in order to be able to discern about the main features of the hemodynamics in the vessel under analysis. For instance, making use of classical "visualization techniques" such as *streamlines*, *iso-surfaces*, *contours* and *glyphs* helps the professional to understand and conclude about the behavior of the complex three-dimensional blood flow taking place in the larger arteries.

Particularly, one of the most relevant hemodynamics factors is related to the *residence time* (see Buchanan et al. (2003); Steinman (2000)). This quantity is attached to all particles in the blood flow, and measures the time they remain in their traveling throughout a certain region of analysis. In other words, they help to characterize stagnation regions by means of the presence of particles with residence times larger than average. The calculation of the residence time for a given particle is, naturally, a Lagrangian concept. Therefore, in order to perform this calculation it is necessary to calculate the pathlines followed by the particles that we want to analyze. This means that we need to carry out particle tracing in order to build the pathlines and to be capable of computing for each particle the corresponding residence time, as well as other quantities of interest such as velocity, and pressure the particle is subjected to along its pathline.

Nevertheless, particle tracing is a tool which is not commonly encountered in open source visualization environments such as Paraview (ParaView, 2009). Then, it is necessary to develop home-made computational implementations so as to do this kind of computations. Since we are dealing with large amount of data resulting from the numerical simulations, such implementations must be efficient, which implies developing parallel implementations.

The simulation of blood flow in arterial vessels poses the problem of performing 3D simulations of incompressible fluid flow in time-varying domains. In addition, the calculation of residence times is strongly dependent of the geometrical features of the vessels, for which the use of patient-specific geometries is compulsory. Furthermore, the embedding of such 3D models into a global 1D arterial network provides a consistent framework so as to carry out numerical simulations considering real physiological regimes for the fluid flow (see Blanco et al. (2007)). The complete scenario can be drawn as follows: (i) reconstruction of the geometrical data from medical images (Magnetic Resonance Imaging and Computed Tomography), (ii) creation of 1D and 3D models, (iii) coupling between the 1D and the 3D model, (iv) numerical simulation, (v) computation of particle pathlines.

This paper presents the development of an efficient computational implementation to perform particle tracing when the input data are velocity fields coming from coupled 3D-1D nu-

merical simulations of blood flow in compliant arteries. Such tool has been integrated into HeMoLab to provide a friendly interface. One of the main features of the present tool, besides its efficiency, lays in the possibility of making particle tracing throughout more than one cardiac beat, although the input corresponds to a unique cardiac cycle. This is essential to compute and study the residence time attached to each particle. This is because usually, geometrical singularities determine large residence times, and more cardiac cycles than expected are needed for the particles to go across a given 3D region. Moreover, the tool provides all the physical quantities of the particles in the flow. For the sake of completeness, some issues concerning the computational implementation in the HeMoLab system are presented and discussed. Also, numerical results are presented to show the usefulness of the tool.

This work is organized as follows: Section 2 presents a brief review of the calculation of particle pathlines, whereas in Section 3 we present the main ideas used for the computational implementation of the tool. Section 4 presents the most important topics about the integration of the tool with HeMoLab, and finally in Section 5 some numerical tests are given. The final comments are presented in Section 6.

2. Basic Review of Particle Tracing

2.1 Basic equations

Particle pathline is a basic concept in fluid mechanics. It arises together with other concepts such as streamlines and streaklines with the aim of characterizing fluid flow. Particularly, pathlines are useful because they allow to study the trajectories of massless fluid particles, as well as to assess the evolution of quantities attached to that given particle throughout the trajectory.

Hence, the computation of particle pathlines implies computing its position, denoted by $\mathbf{x}$, as a function of time. The velocity field that describes the flow in Eulerian form is denoted by $\mathbf{v}$, which is a function of the position $\mathbf{x}$ and time t. The Lagrangian counterpart of the velocity field is denoted by $\mathbf{v_p}$, which is a function of the particle, denoted by $\mathbf{p}$, and of time t. Therefore, the problem can be mathematically written as follows: given a particle identified by its initial position, say $\mathbf{p}$, with velocity $\mathbf{v_p}(\mathbf{p}, t)$, find $\mathbf{x_p} \in \mathbb{R}$ solution of the initial value problem

$$\begin{cases} \frac{d\mathbf{x_p}}{dt} = \mathbf{v_p}(\mathbf{x_p}, t) \quad t \in [t_0, T_\mathbf{p}], \\ \mathbf{x_p}|_{t=t_0} = \mathbf{p}, \end{cases} \tag{1}$$

where, as said before, $\mathbf{p}$ is the ID of the particle, which coincides with its initial position at t_0, and $T_\mathbf{p}$ is the final time for which the trajectory of particle $\mathbf{p}$ was computed. In our application, for a given region of analysis, say Ω, each particle is released from an initial position until it, eventually, goes out of such a domain. Thus, for each particle we have that the time it remains in the domain of analysis is given by $T_\mathbf{p}$. With this concept, we define the residence time of each particle as the time $T_\mathbf{p}$ it tooks to particle $\mathbf{p}$ to cross the whole domain Ω.

Notice that here we are dealing with a Lagrangian analysis, then we are able to study the state of the particles concerning their velocity field (which is intrinsically needed by the pathlines calculation process) and their pressure state. More generally, we can analyze the whole stress state of each particle along its trajectory.

In the examples studied here, the blood flow velocity is derived from numerical simulations of Newtonian flow in three-dimensional domains. The mathematical model is briefly described later on.

2.2 Relevance in computational hemodynamics

Pathlines computation is important in computational hemodynamics because computing the pathlines of blood particles helps to understand the complex patterns of blood flow in real patient-specific geometries. As a matter of fact, it is believed that chemical interactions between the arterial wall and the suspensions in the blood flow lead to wall thickening, one of the major causes of artery occlusion (Buchanan et al., 2003). Another instance is the pressure the particles are subjected to. Indeed, it is believed that particles with high exposure time to low pressure might result in cavitation phenomena, leading to arterial wall damage (Brujan, 2009). All these phenomena are strongly related to high residence times, which are, in turn, result of stagnations regions within the arterial vessel. This is the context that motivates the development of tools to compute the trajectories of a set of particles in the blood flow.

3. Efficient Parallel Implementation of Particle Tracing Algorithms

In the present section, the main elements involved in the implementation of a parallel computational implementation for performing particle tracing are described.

Previously on (Porto et al., 2004), the problem of computing efficiently particle pathlines was addressed. In the present implementation, the input datasets of this system included information about fluid particles' initial position, the geometry of the cell domain decomposition and fluid velocity vectors associated with the cell's vertices (Hamann et al., 1995). These datasets were modeled by means of the following relations.

1. Particles (part-id, time-instant, point): particles in their initial position in an instant.
2. Geometry (id, point): cell domain decomposition.
3. Velocity (point, time-instant, intensity): the velocity of fluid in cell vertices.

In addition, a program trajectory (particle-id, point, velocity) that computes the next position of a given particle was considered, producing a tuple (particle-id, point). The computation of particle paths consists of registering particles' positions at each time step.

Large datasets make the search of the appropriate velocity vectors a very intensive computational task. To reduce the time spent on searching, the input dataset must be partitioned. This way, a preprocessing step is required to find in which partition one specific particle must be processed each time.

In this implementation, the data was partitioned in several clusters called *Meta-Cells*. Meta-cells are constructed following the steps below:

- Sort all data points by the x-values, and partition them into H consecutive chunks;
- For each such chunk, sort its data points by the y-values, and partition them into H consecutive chunks.
- For each such chunk, sort its data points by the z-values, and partition them into H consecutive chunks.

Each particle's position is calculated by finding in which meta-cell it is currently contained. When a particle is positioned between two or more meta-cells, they are all considered to define the new position of the given particle.

4. Implementation Issues on top of ParaView

The Paraview environment has a very limited support for particle tracing methods. Several issues as data reading and transfer of all the time steps, the development of a intuitive user interface for positioning the set of particles, the repetition of the cardiac pulse and the computation of intermediate time steps were addressed and will be presented in the following subsections.

4.1 User Interface

The Particle Tracing filter has the following workflow:

- Open the initial set of files. The files must be in *EnSight* (International, 2009) format;
- Select the *HM 3D Particles Tracing Filter* of the *Filter* menu;
- Configure the parameters (output directory, particle's radius, quantity and initial position, number of repetitions of the cardiac pulse and the insertion of new time steps);
- Press the *Accept* button to apply the filter;
- Press the *Play* button of the animation bar;

The output of the filter is a *EnSight* file and will be stored in the directory selected by the user.

The widgets help the positioning and configuration of the set of particles that will be traced. The positioning is performed intuitively using the *mouse* device. The interface has three different *widgets* as follow:

- *Points Cloud* - Creates a cloud of n points (where n is the number of particles) with a parameter to set the maximum distance between each point and the center of the cloud.
- *Line* - Creates a line and set n particles over it
- Sphere - Creates a random distribution of particles inside a parameterized sphere. The user interface is composed by the center and radius of the sphere and the number particles that will be created.

4.2 Additional Tools

The input files usually have just one cardiac cycle and sometimes a specific particle requires more cycles to pass through a structure like an artery. For this reason, methods to replicate cardiac cycles were created. The user informs the number of cardiac cycles that will be used during the particle tracing processing.

To reduce the differences between the position of the particles in each time step, interpolation methods where used to produce a new set of positions.

5. Numerical Results

In the first part of this section the model used in the numerical simulations to compute the velocity vector field is briefly described. Then, such model is employed to study the blood flow in two situations: (i) hemodynamics in a cerebral artery with an aneurysm and (ii) hemodynamics in a healthy iliac bifurcation. These two simulations are taken from previous works, see (Blanco et al., 2009) and (P.J. Blanco and M.R. Pivello and S.A. Urquiza and N.A. de Souza e Silva and R.A. Feijóo, 2009), respectively. Therefore, no further comments regarding the details of the physiological values and numerical parameters are given.

5.1 Mathematical model for blood flow

As already said in a previous section, the particle tracing filter is fed with a three-dimensional time-varying velocity field. This vector field is obtained from a numerical simulation. Within the HeMoLab system, the simulations are performed following a 3D-1D coupled approach (see Blanco et al. (2007)). That is, 1D models of fluid flow in compliant vessels are coupled with the full three-dimensional Navier-Stokes equations in order to take into account the systemic interactions between the different scales within the arterial network. In this manner, it is possible to carry out simulations in real physiological regimes, with all its implications. This is relevant when thinking of computing particle trajectories and the pressure state of those particles. In fact, small disturbances in eventual boundary conditions, obtained, for instance, from measurements (in the case of using standalone 3D models) can lead to great differences in the velocity field, with its natural outcomes.

The associated Euler equations for a Newtonian fluid when coupling a 1D model defined in a 1D domain Ω_{1D} with a 3D model defined in the region Ω_{3D} through a coupling interface Γ_c, and considering the ALE (Arbitrary Lagrangian Eulerian) formulation over Ω_{3D}, are the following:

$$\rho A\frac{\partial \bar{u}}{\partial t}+\rho A\bar{u}\frac{\partial \bar{u}}{\partial z}=-A\frac{\partial \bar{p}}{\partial z}-8\pi\mu\bar{u}+f^z \qquad \text{in } \Omega_{1D}\times(0,T) \tag{2}$$

$$\frac{\partial A}{\partial t}+\frac{\partial\left(A\bar{u}\right)}{\partial z}=0 \qquad \text{in } \Omega_{1D}\times(0,T) \tag{3}$$

$$\rho\left.\frac{\partial \mathbf{u}}{\partial t}\right|_{\mathbf{Y}}+\rho\nabla\mathbf{u}\left(\mathbf{u}-\mathbf{w}\right)=-\nabla p+\mu\Delta\mathbf{u}+\mathbf{f} \qquad \text{in } \Omega_{3D}\times(0,T) \tag{4}$$

$$\nabla\cdot\mathbf{u}=0 \qquad \text{in } \Omega_{3D}\times(0,T) \tag{5}$$

$$\left(-p\mathbf{I}+2\mu\boldsymbol{\varepsilon}(\mathbf{u})\right)\mathbf{n}_1=-\bar{p}\mathbf{n}_1 \qquad \text{on } \Gamma_c\times(0,T) \tag{6}$$

$$A_c\bar{u}=\int_{\Gamma_c}\mathbf{u}\cdot\mathbf{n}_1\,d\Gamma \qquad \text{on } \Gamma_c\times(0,T) \tag{7}$$

Where $\mathbf{n}_1$ is the unit outward normal to domain Ω_{1D} over the coupling interface Γ_c. Equations 2 and 3 represent the 1D model, where $\bar{u}$ and $\bar{p}$ are the mean velocity and pressure values, ρ is the blood density, μ is the dynamic viscosity, A denotes the cross sectional area, $Q=A\bar{u}$ is the flow rate and z is the axial coordinate. Equations 4 and 5 stand for the 3D model, where $\mathbf{u}$ is the blood velocity, $\mathbf{w}$ is the domain velocity of change consistent with the ALE framework, while p is the blood pressure. Equation 6 gives the continuity of the traction vector at Γ_c, whereas expression 7 is the counterpart of the mass conservation.

The arterial wall is modelled using an independent ring model (Kivity and Collins, 1974), that is

$$\bar{p}=\bar{p}_0+\frac{E\pi R_0h_0}{A}\left(\sqrt{\frac{A}{A_0}}-1\right)+\frac{k\pi R_0h_0}{A}\frac{1}{2\sqrt{A_0A}}\frac{\mathrm{d}A}{\mathrm{d}t} \qquad \text{in } \Omega_{1D}\times(0,T) \tag{8}$$

$$p=p_0+\frac{Eh}{R_0^2}\zeta+\frac{kh}{R_0^2}\frac{\mathrm{d}\zeta}{\mathrm{d}t} \qquad \text{in } \Gamma_w\times(0,T) \tag{9}$$

Finally, the deformation of the domain Ω_{3D} is accounted for through a Laplacian problem, as stated below

$$\nabla^2\mathbf{d}=0 \qquad \text{in } \Omega_{3D}\times(0,T) \tag{10}$$

Equation 10 is used to extend the wall displacement to the interior of Ω_{3D}, and $\mathbf{d}|_{\Gamma_w} = \zeta \mathbf{n}$ is the wall displacement, where ζ is the scalar field that denotes the displacement of the wall in the normal direction, given by $\mathbf{n}$, that is obtained from equation 9. Finally, it is $\mathbf{w} = \frac{\partial \mathbf{d}}{\partial t}$. Refer to (Blanco et al., 2007) for a further theoretical account about the coupling of 3D-1D blood flow models.

5.2 Particle tracing in the cerebral artery

This first example aims at presenting the results of blood flow particle tracing in a cerebral artery in the presence of a geometrical perturbation which emulates an aneurysm. This simulation involves a three dimensional discretization of the domain rendering 81000 nodes and a time discretization such that each cardiac cycle, with period $T = 0.8$ sec, is divided into 640 time steps, from which just 160 time steps are used in the calculation of particle pathlines. In Figure 1 the geometry and the solution (flow and pressure curves) at both coupling interfaces are presented. Such solution is attained after solving the coupled 3D-1D problem. In that figure, the solutions at the coupling interfaces are given for both cases, with aneurysm (as in the present study) and without the aneurysm.

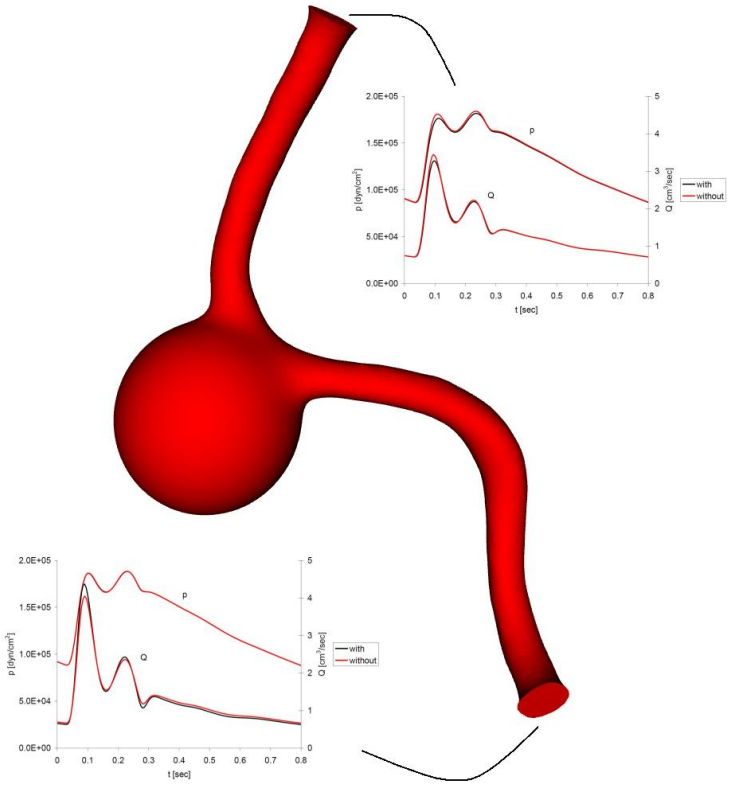

Figura 1: Geometry of the cerebral artery with an artificially created aneurysm and solutions at the coupling interfaces.

The periodic state is reached after three cardiac beats. Then, the last beat is used as the input for the particle tracing algorithm. Since the particles are expected to remain in the domain of analysis more than a cardiac period the particle tracing filter is set to perform the pathlines computation throughout three cardiac beats. In this case, 100 blood particles randomly placed within a sphere widget are released near the proximal coupling interface. Figure 2 presents the a detail of the particle trajectories at the end of the three diastolic phases. The pathlines are colored with the magnitude of the velocity field.

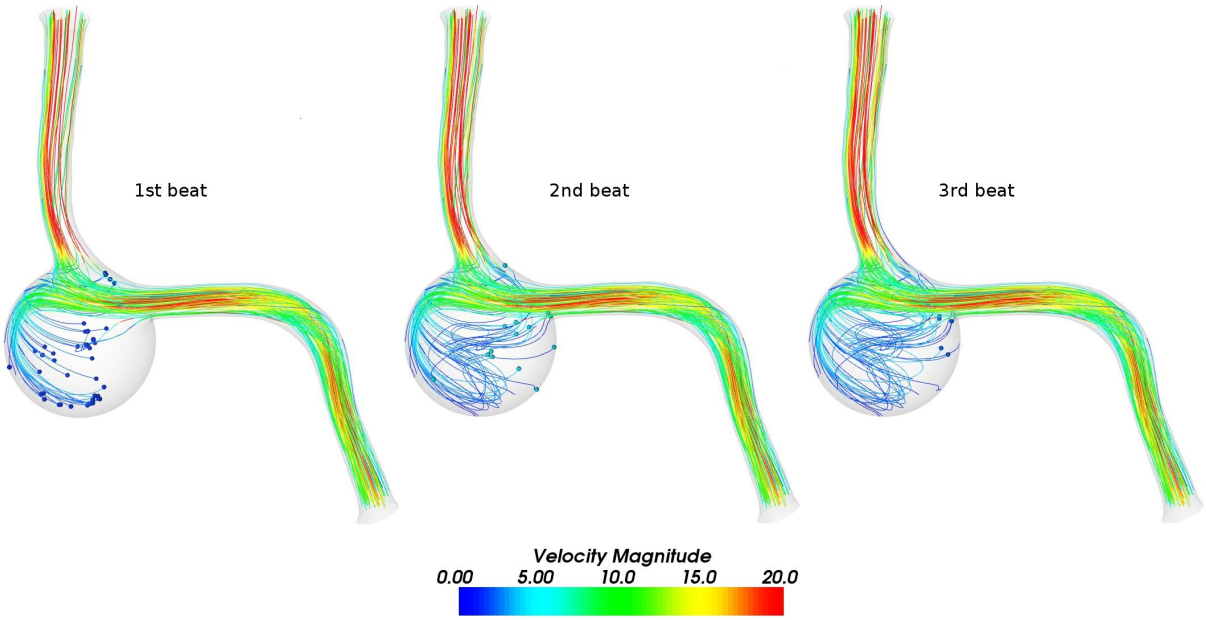

Figura 2: Particle trajectories at the end of diastolic phases.

In turn, Figure 3 shows the trajectories after the three cardiac beats and other details. Notice that due to the geometrical features of the vessel, even after three beats (that is 2.4 sec.) we have particles in the intra-aneurismal region. In this case, the pathlines pattern is colored with the value of the residence time. In this way, observe that there is about 20% of particles which remains in the region of analysis more than two beats. This kind of results helps to understand the complex blood flow patterns induced by an aneurysm-like geometrical singularity.

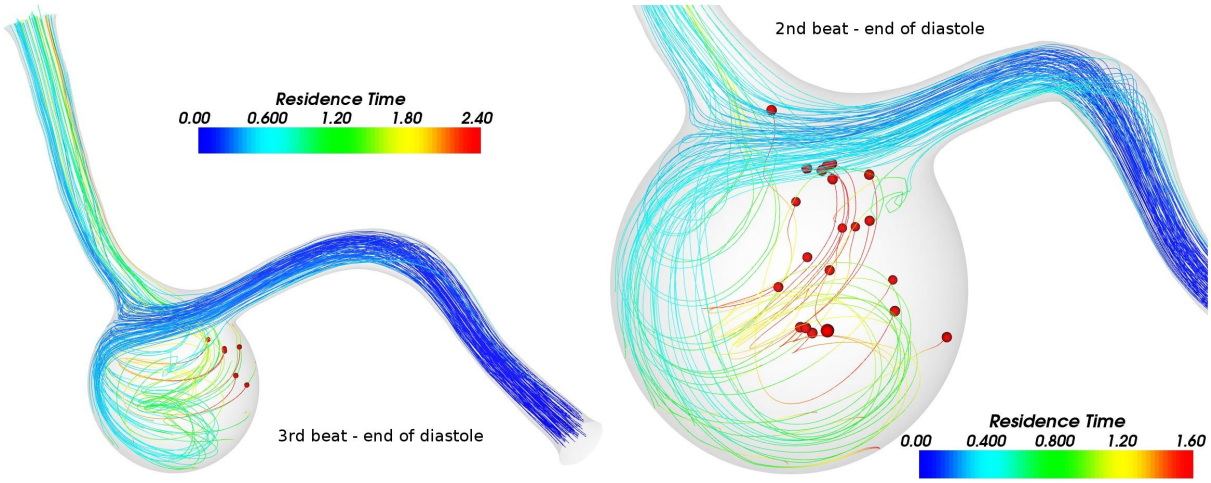

Figura 3: Detail of pathlines and residence time for different time instants.

which enter in the intra-aneurysmal region

5.3 Particle tracing in the abdominal aorta artery

In this second example we perform a rather more expensive computation. The particle tracing algorithm is used to study the blood flow in the abdominal aorta artery including the iliac bifurcation. The computational fluid dynamics simulation was carried out with a mesh containing 545000 nodes, while the time discretization (for a period $T = 0.8$ sec) resulted in 640

time steps, from which, again, just 160 time steps are used in the calculation of the trajectories. Figure 4 shows the geometry of the vessel under analysis and the global information, given by flow rate and pressure, at the coupling interfaces. Recall that these curves are obtained from the 3D-1D simulation.

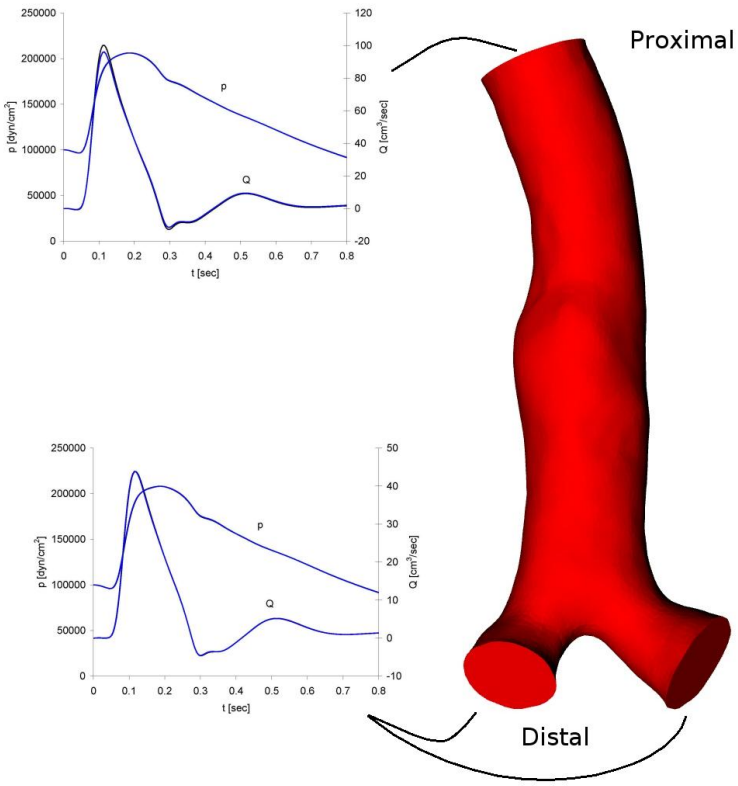

Figura 4: Geometry of the abdominal aorta and solutions at the coupling interfaces.

In this case, two cardiac beats are simulated, and the second one is considered as the periodic state. This beat is employed as the input for the particle tracing algorithm which, in turn, is repeated four times to generate four consecutive beats. In this case, the pathlines of 200 blood particles along these four cardiac cycles are computed. They are randomly released in the blood flow at the entrance of the domain, at the proximal side. In figure 5 an image sequence of the trajectories is shown. The four images represent two time instants, at systole and at diastole, for the first two beats. The pathilnes are colored with the value of the pressure. This makes easy the identification of the global state with respect to systolic/diastolic pressures, that is, it helps to analyze in which periods the particles are subjected to high and low pressure values.

In Figure 6 a detail of the pathlines in the middle area of the vessel is shown. This result corresponds to the late part of the diastolic phase in the first beat. Notice the intricacy of the pathlines as a result of the mild curvature and mild enlargement of the arterial geometry. This tells us about the high sensitivity of fluid behavior with respect to the geometrical features of real vessels. This is relevant in determining the residence time of the particles. In fact, in Figure 7 we observe the pathlines that now are colored with the residence time. Note that, even after three cycles, there are regions with particles (in red). These particles have a residence time higher than 2.0 sec. Specifically, about 10% of the released particles remain more than three cardiac beats, something that provides a concrete characterization of blood flow with the purpose of integrating numerical simulations and medical research.

This kind of result helps to understand the complex blood flow patterns induced by a geo-

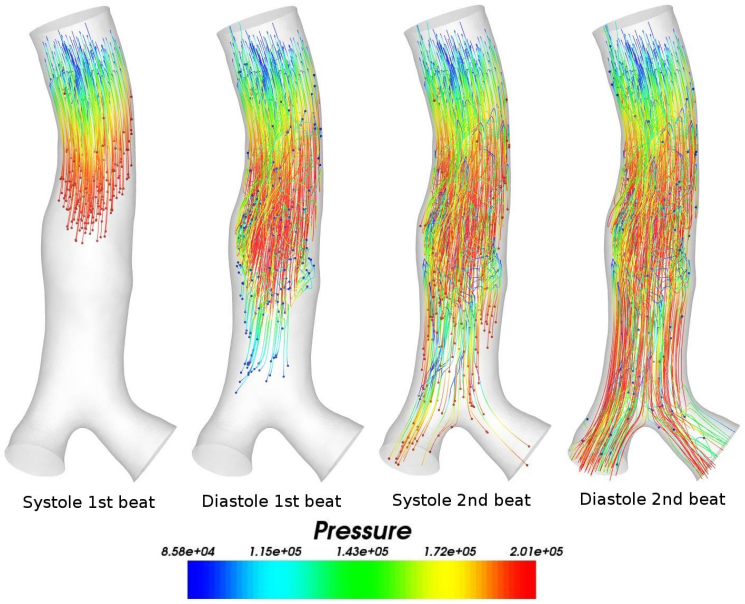

Figura 5: Particle pathlines in the first and second cardiac cycles.

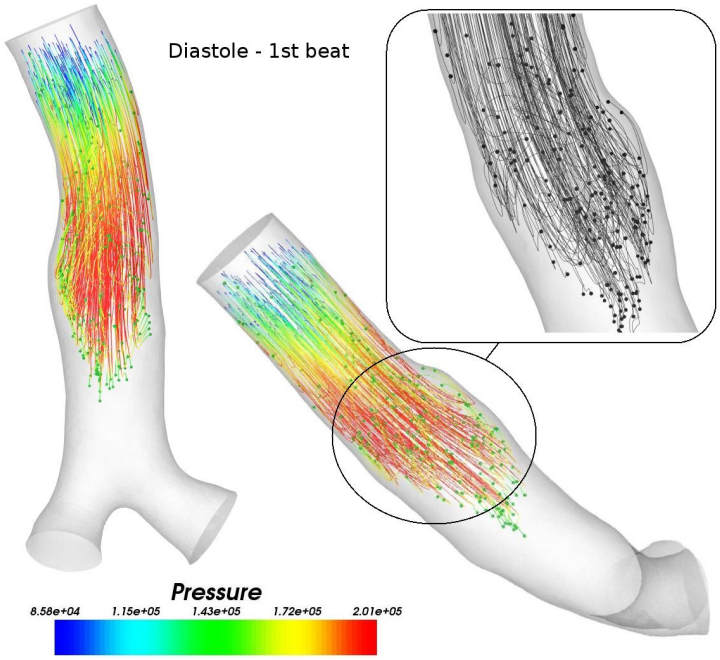

Figura 6: Detail of pathlines at the middle area of the vessel.

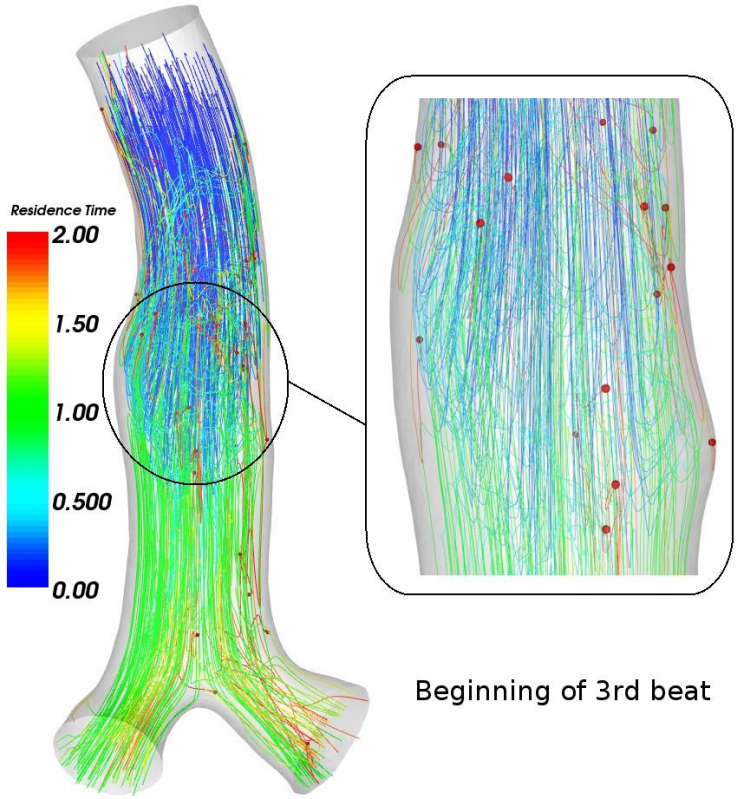

Figura 7: Pathlines after three cardiac beats.

metrical irregularities, which are commonplace in arterial vessels. Indeed, one of the the next steps towards combining computational hemodynamics and cardiovascular research could be the association of the large residence times observed in particles with chemical interactions between particles and arterial wall.

6. Final Remarks

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