Numerical Modeling of Nanoparticles Tracking

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Abstract. A 3D computer simulation of blood flow with a magnetic component was developed in the diffuse programing environment ROOT. The simulation allowed us to calculate the force on particles in the blood, and to find the conditions under which it is possible to confine them in a desired area, for instance for safe and therapeutic release of medical products.

Introduction

Mathematical operations and data processing can be significantly accelerated by using local cluster of tens of PCs or a GRID consistings of several hundred computers. Such facilities can reduce calculations from several weeks to few days or even hours. The most time-consuming mathematical and physical operations include, among others, calculations in the biomedical field. Magnetic nanoparticles as well as magnetic fluids, which are precursors of nanotechnology, are now often used in different contexts. They are now widely used in various fields of physics, technology and medicine. Applications of magnetic fluids are based on the possibility to modify their properties under the influence of a magnetic field, at the same time using their liquid properties. In the biomedical field it is possible to use the transport of targeted drugs, either in magnetic hyperthermia or in radiodiagnostics. This method can be applied in magnetic resonance studies to contrast media in the orientation of biological systems, cellular and biomolecular bio-magnetic separation even in sewage treatment. Present attention in biomedicine and biophysics focuses on cell separation, targeting of drugs and the application of magnetic fields to separate cells.

The goal of our work is that we developed a computer simulation using ROOT to study the transport of a magnetically labeled drug inside the blood system. This was done by calculating the force acting on these particles and to find the conditions under which it will be possible to capture the transported material at the desired location, so that medical effect is optimized. Since these simulations are time-consuming, we performed these with ROOT using the GRID and PC cluster.

Numerical Modeling of Nanoparticles in the Blood Stream

To be able to describe the dynamics of the moving particles within a magnetic field, we study the forces that act between the particles. Experiments show that these forces are different following from Coulomb’s law. Therefore, in the past for these cases, formulated new laws – moving particles generate an electric field outside the box and showing other characteristics, i.e., magnetic field. The motion of magnetic nanoparticles in the blood stream under the influence of magnetic field was studied for 2D case in papers [1, 2, 3]. Equation in general terms looks:

\begin{equation}
m_p \frac{d^2 \vec{R}}{dt^2} = \vec{F}_{\text{mag}} + \vec{F}_{\text{drag}},
\end{equation}

where \( \vec{R} \) is the radius vector of the nanoparticle, \( m_p \) is the mass of particles \( \frac{4}{3} \pi r^3 \rho \), where \( \rho \) is the density of magnetically labeled particles \( \vec{F}_{\text{mag}} \) force acting upon the nanoparticles by the magnetic field, \( \vec{F}_{\text{drag}} \) is the drag force. The movement of particles will be modelled by solving the Cauchy problem within a rectangular coordinate system \((Oxyz)\), where the drag force is expressed as follows:

\begin{equation}
\vec{F}_{\text{drag}} = -6 \pi \eta R_p \left( \frac{d\vec{R}}{dt} - \vec{v}_b \right),
\end{equation}

The vector equation can be rewritten using the Cartesian coordinate system. In the 3D Cartesian coordinate system can be this system expressed:

\begin{align*}
& m_p \frac{d^2 x}{dt^2} = -6 \pi \eta R_p \left( \frac{dx}{dt} - v_{xb} \right) - \\
& - \frac{\chi V_x}{\mu_0} \left( B_x \frac{\partial B_x}{\partial x} + B_y \frac{\partial B_y}{\partial y} + B_z \frac{\partial B_z}{\partial z} \right), \\
& m_p \frac{d^2 y}{dt^2} = -6 \pi \eta R_p \left( \frac{dy}{dt} - v_{yb} \right) - \\
& - \frac{\chi V_y}{\mu_0} \left( B_x \frac{\partial B_x}{\partial x} + B_y \frac{\partial B_y}{\partial y} + B_z \frac{\partial B_z}{\partial z} \right), \\
& m_p \frac{d^2 z}{dt^2} = -6 \pi \eta R_p \left( \frac{dz}{dt} - v_{zb} \right) - \\
& - \frac{\chi V_z}{\mu_0} \left( B_x \frac{\partial B_x}{\partial x} + B_y \frac{\partial B_y}{\partial y} + B_z \frac{\partial B_z}{\partial z} \right).
\end{align*}

\begin{itemize}
\item \( \eta \) – the density of blood;
\end{itemize}
• $R_p$ – the radius of particle;
• $\vec{R}$ – the radius vector;
• $v_b$ – the speed of blood;
• $\chi$ – the magnetic susceptibility;
• $\vec{B}$ – the magnetic induction;
• $V_p$ – the volume of particles $\frac{4}{3} \pi R_p^3$

**Simulation and Analysis of Tracks**

This task was divided into the following two parts. The simulation of tracks was performed in the first part, while in the second part the analysis of the resulting tracks was performed. Since the path simulation of one particle takes about 6 seconds, the GRID comprising of 100 PCs was used, which on each PC 1000 tracks (were simulated). Since this task was performed sequential, the total simulation lasted 3 hours and 25 minutes. Each “worker” on the GRID produced a set of one thousand tracks, which were then copied to the PROOF cluster. Using packages on PROOF we analyzed each track in parallel. The present simulation results are comparable with results obtained in [1], which used an analytical method for calculating the trajectories of nanoparticles under the influence of the magnetic field generated by a cylindrical magnet. It is noteworthy that our model is developed based on numerical simulations which allow us to present 3D particle trajectories under the influence of the magnetic field and the function known in advance that we can point in any component $B_x(x, y, z)$, $B_y(x, y, z)$, $B_z(x, y, z)$ magnetic field or it will be necessary to obtain this function using the method of least squares from the map of the magnetic field.

Specifically for our model vein, we used the following parameters: $v_b$ is the velocity of blood, $R_p$ is the radius of the magnetically labeled particles, vein length is 20 cm, magnetic field is $[-3, 3]$, where we then chose the handle area $[-1, 1]$. The results of simulations and subsequent analysis at different radii and speed of magnetic nanoparticles are shown in (Table 1). To view a sample collected just handle simulations of magnetically labeled particles in a chosen field.

Fig. 1 shows the tracks of magnetic particles with a radius of $500 \cdot 10^{-9}$ [m] and an initial track speed of $1 \cdot 10^{-3}$ [m·s$^{-1}$] from an external perspective and view of the magnet. As well as the upper images display a red vein, a gray square shows the magnet, and the actual path of magnetic particles are shown in gray [5].

**Conclusion**

In this article a 3D computer simulation of blood flow with a magnetic component in diffuse programming environment ROOT was developed. In frames of this simulation the force acting on the magnetic particles was calculated and the conditions needed for capture and keep of these particles in desired area were estimated. In our model for used initial condition (velocity of blood, radius of magnetically labeled nanoparticles) the trajectory of nanoparticle can be estimated. To establish these conditions are very important as during the keeping the drug immobilized on magnetic nanoparticles can be released and so satisfied their therapeutic role.

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