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FAST COMPUTER SIMULATION METHOD OF THROMBUS FORMATION ON PIPE ORIFICE FLOW

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Abstract. *This paper presents the performance of the parallel algorithm for simulating thrombus formation on pipe orifice flow by using a PETSc software library package. Since the computational cost for bio-fluid problems is very expensive, an efficient algorithm such as parallel computing is necessary in order to overcome this limitation. The parallel program reduces the computational time by dividing workload to calculate simultaneously for each processor or computer. This will help researchers and physicians for medical diagnosis and development of medical devices. The blood flow used in this analysis is modeled by the incompressible Navier-Stokes equations with a partially patched modified* $k - \epsilon$ *model. Moreover, the platelet adhesion model is used for predicting the formation of thrombus. We perform the numerical experiments on the orifice configuration. The results show that our program can reduce the computation time by increasing the number of processors.*
Keywords: Thrombus formation, Parallel programming, CFD

1. **Introduction.** In these days, the development of medical technology is growing continuously. One of the important medical devices is an artificial organ, especially rotary blood pump. However, there is a chance to occur blood clot or thrombus in the pump. In order to prevent this condition, understanding of the thrombus formation by flow field is necessary. Moreover, the prediction of the thrombus growth is also important for designing the medical appliances with blood flow.

There are numerous computational models used for representing various aspects of blood flow and thrombus formation [1-3]. These models are helpful tools for researchers and physicians to understand a vascular system and provide the important information for better diagnosis and treatment. In order to evaluate and simulate these flow problems, computational fluid dynamics (CFD) analyses have been used.

Since the bio-fluid problems such as previous works [4,5] are complicated, the computational cost is very expensive. In order to achieve a better solution, an efficient algorithm such as parallel computing is required. The parallel computing is a simultaneous process for performing large or intensive computational problems. This method will divide the task into small tasks that can be solved simultaneously using multiple processors or computers. This approach will obviously obtain the results faster. In [6,7], they applied the parallel algorithm for solving the incompressible Navier-Stokes equations. However, their

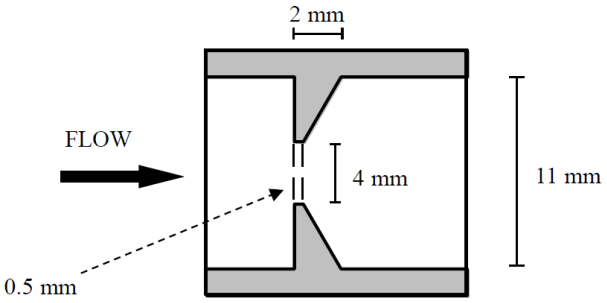

FIGURE 1. Schematic geometry of the orifice configuration for our experiment

works do not include the transport equations of turbulent energy and energy dissipation. Thus, their results are not reasonable when Reynolds number is getting bigger.

In this paper, we aim to present the performance of the parallel algorithm for simulating thrombus formation on pipe orifice flow (Figure 1) using Portable, Extensible Toolkit for Scientific Computation (PETSc) software package. The flow model used in this analysis is defined by the incompressible Navier-Stokes equations and the transport equations of turbulent energy and energy dissipation (a partially patched modified $k-\epsilon$ model) [3]. The platelet adhesion model [8] is used to predict the formation of thrombus. In addition, we use a domain decomposition method to divide the problem into several subdomains in order to solve the thrombus formation model in [8]. The solution obtained by this approach is efficient in terms of the computational time. Furthermore, the results of the thrombus formation with and without using the Navier-Stokes equations and the turbulent transport equations are compared.

This paper is organized as follows. The introduction is presented in Section 1. The blood flow model and the thrombus formation model for our experiments are presented in Section 2 and Section 3, respectively. Section 4 focuses on the domain decomposition method. The numerical results and discussion are presented in Section 5. Finally, conclusion is presented in Section 6.

2. **Blood Flow Model.** The blood flow models used in this paper are dimensionless incompressible Navier-Stokes equations and the transport equations of turbulent energy k and energy dissipation ϵ in a cylindrical coordinate as follows:

$$\frac{\partial u}{\partial x}+\frac{1}{r}\frac{\partial (rv)}{\partial r}=0 \tag{1}$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial r}=-\frac{\partial p}{\partial x}+\left(\frac{1}{\mathrm{Re}}+v_t\right)\nabla^2 u+2\frac{\partial v_t}{\partial x}\frac{\partial u}{\partial x}+\frac{\partial v_t}{\partial r}\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial x}\right) \tag{2}$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial r}=-\frac{\partial p}{\partial r}+\left(\frac{1}{\mathrm{Re}}+v_t\right)\left(\nabla^2 v-\frac{v}{r^2}\right)+2\frac{\partial v_t}{\partial r}\frac{\partial v}{\partial r}+\frac{\partial v_t}{\partial x}\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial x}\right) \tag{3}$$

$$\frac{\partial k}{\partial t}+u\frac{\partial k}{\partial x}+v\frac{\partial k}{\partial r}=\frac{1}{\mathrm{Re}}\nabla^2 k+\frac{1}{\sigma_k}\left(\frac{\partial v_t}{\partial x}\frac{\partial k}{\partial x}+\frac{\partial v_t}{\partial r}\frac{\partial k}{\partial r}\right)+G-\epsilon \tag{4}$$

$$\frac{\partial \epsilon}{\partial t}+u\frac{\partial \epsilon}{\partial x}+v\frac{\partial \epsilon}{\partial r}=\frac{1}{\mathrm{Re}}\nabla^2 \epsilon+\frac{1}{\sigma_\epsilon}\left(\frac{\partial v_t}{\partial x}\frac{\partial \epsilon}{\partial x}+\frac{\partial v_t}{\partial r}\frac{\sigma\epsilon}{\partial r}\right)+C_{\epsilon 1}\frac{\epsilon}{k}G-C_{\epsilon 2}f_\epsilon\frac{\epsilon^2}{k} \tag{5}$$

$$v_t=C_\mu f_\mu\frac{k^2}{\epsilon},\quad G=v_t\left[2\left\{\left(\frac{\partial u}{\partial x}\right)^2+\left(\frac{\partial v}{\partial r}\right)^2+\left(\frac{v}{r}\right)^2\right\}+\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial x}\right)\right] \tag{6}$$

where u is the velocity in x-direction (along pipe), v is the velocity in r-direction (radial position), p is the pressure, Re is the Reynolds number, and f_ϵ and f_μ are damping functions. Equations (1)-(6) are the Navier-Stokes equations and the transport equations of turbulent energy and energy dissipation. In this paper, these equations are called NST.

3. **Thrombus Formation Model.** In this analysis, we consider the formation of thrombus in terms of platelet adhesion model proposed by Babushkina et al. [8] in the dimensionless form as follows.

$$\frac{\partial C}{\partial t} = k_{adh}\gamma(1-C)\left(\frac{C}{\gamma}+|\nabla C|\right) - k_{rol}\left(u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial r}\right) \tag{7}$$

where C is the concentration of adhered platelets, γ is the wall shear rate, k_{adh} is the platelet adhesion efficiency rate constant, and k_{rol} is the platelet movability within thrombus rate constant. When the concentration C is bigger than proper value of concentration C_B ($C > C_B$), the platelet will adhere to the wall and become a part of thrombus. The assumption of this model is that the thrombus is solid so that the fluid cannot permeate. As a result, the velocities of fluid inside this area are zero.

We also set the initial concentration of platelet to be one at the wall near the reattachment point and in front of the contraction part of configuration in accordance with the results from [9] which shows that the high concentration always occurs in these regions. As for the boundary conditions, we choose the inlet boundary to be zero and use zero gradient boundaries for the outlet and the wall.

4. **Domain Decomposition Method.** Domain decomposition method [10] is the method to solve the problem by partitioning the domain of the problem into several subdomains and calculate collaboratively over these subdomains in order to solve the problem faster. Figure 2 illustrates the domain decomposition methodology. The domain is discretized into grid points as shown in Figure 2(A). Then the model is partitioned into subdomains, for example, four subdomains as shown in Figure 2(B). Each subdomain will be calculated simultaneously and independently on each processor. However, at the boundary, they require the information of adjacent points which are owned by neighboring processors. To access these values, the ghost points are defined at the adjacent points of subdomain for each processor. Figures 2(C)-2(F) show the ghost points (cross symbols) in processor 0-3, respectively. These ghost points are needed to update values before the next time step. This procedure allowed the communication between each processor.

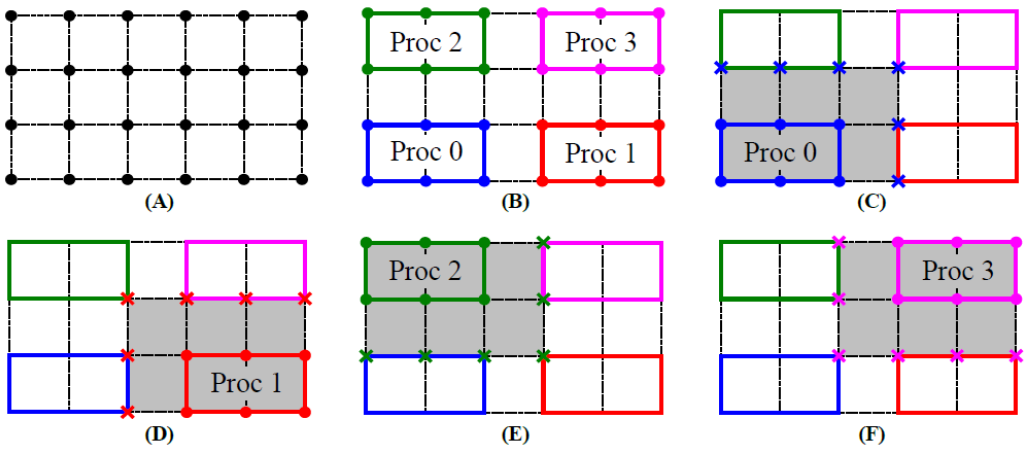

FIGURE 2. Domain discretizing and the box-type stencil ghost points (cross symbols)

5. **Numerical Results and Discussions.** In this section, we perform the numerical simulations of thrombus formation on pipe orifice flow. The program is written in C language using PETSc 3.6.3 software library and run in parallel on a computer with Intel Core i7-3770 CPU, 16 GB RAM, and Windows 7 64-bit operating system. Reynolds number used in this analysis is 5,000 and the time step is 0.00001. The values of parameters used in the Navier-Stokes equations and the platelet adhesion model are as follows:

$C_\mu = 0.09$, $C_{\epsilon 1} = 1.5$, $C_{\epsilon 2} = 1.9$, $\sigma_k = 1.4$, $\sigma_\epsilon = 1.4$, $k_{adh} = 4 \times 10^{-9}$, $\lambda = 1.5 \times 10^{-4}$, and $k_{rol} = 7 \times 10^{-5}$. The threshold level of concentration C_B is assumed to be 0.9. Thus, the platelet becomes thrombus when it reaches this level.

Since the computational time for solving NST has high cost, it is a good idea to investigate the effect of NST on the thrombus formation. Figure 3 presents the tendency of thrombus growth with and without using NST. Equations (1)-(7) are solved numerically in the model with using NST, while only Equation (7) is solved using the value of fluid velocity at the statistically steady state (i.e., the average of flow field does not change in time) in the model without using NST. The results show that, at time step $t = 10000$, there is no development of the thrombus in the model using NST. However, in the model without using NST, the thrombus begins to develop at the contraction part. For both models, the thrombus develops from the wall and moves to the contraction area when $t = 30000$. We can see that the results, between the models with and without using NST, are quite similar. The comparison of CPU time at 10^6 iterations is demonstrated in Figure 4. The results show that the computational time of the model without using NST is around 1/15 of the time in the model using NST.

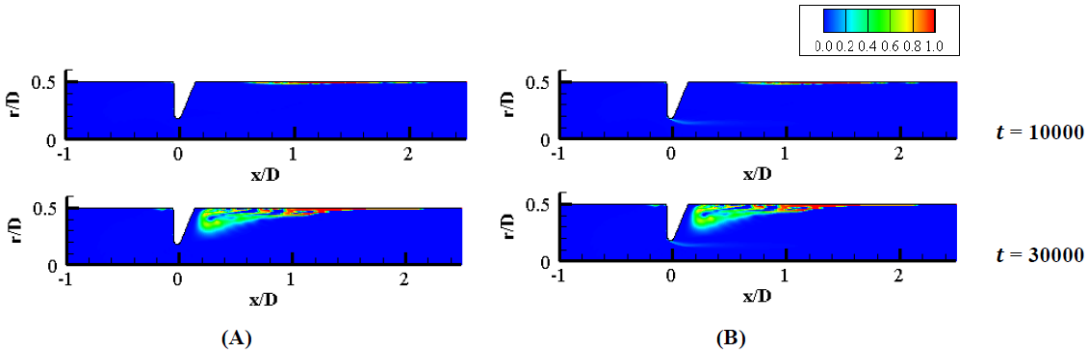

FIGURE 3. The distribution contours of concentration (A) with using NST and (B) without using NST at $t = 10000$ and 30000

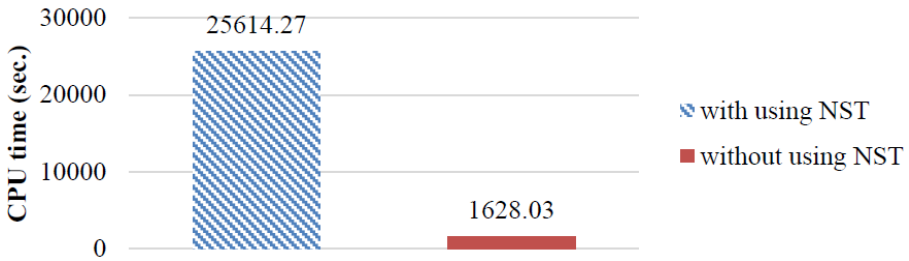

FIGURE 4. Comparison of CPU time at 10^6 iterations

To further overcome the limitation of the computational cost, the parallel algorithm is applied by using the domain decomposition method as shown in Section 4. Figures 5(A) and 5(B) show the speedup and the efficiency of the parallel algorithm, respectively. The definitions are defined as follows:

$$S(n) = \frac{T(1)}{T(n)} \qquad E(n) = \frac{S(n)}{n} \tag{8}$$

where $S(n)$ and $E(n)$ are the speedup and the efficiency of the n processors parallel algorithm, respectively. $T(1)$ is the computational time of the 1 processor (sequential) algorithm, and $T(n)$ is the computational time of parallel algorithm executed on n processors.

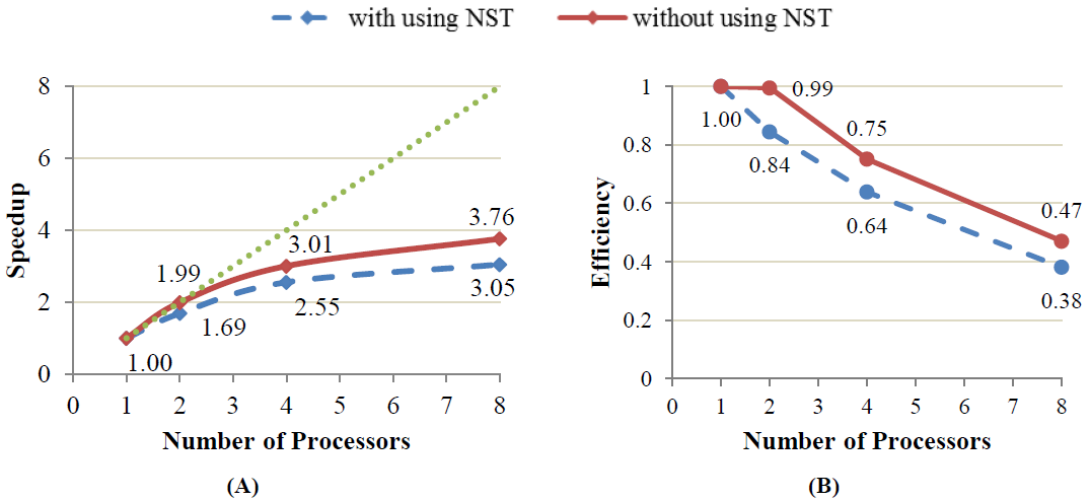

FIGURE 5. (A) Speedup and (B) efficiency of the parallel algorithm

Figure 5(A) shows the speedup of the parallel program using 1, 2, 4, and 8 processors, respectively. We can see that, as the number of processors increases, the speedup rises (the computational time reduces). However, when we increase the number of processors, the efficiency of our program decreases as shown in Figure 5(B) because there is more communication between each processor. In addition, the less communication between each processor of the model without solving NST result in the better speedup and efficiency compared with the model using NST.

6. **Conclusion.** In this paper, we have presented the performance of the parallel algorithm for simulating thrombus formation on pipe orifice flow. The main purpose of this developed algorithm is to reduce the computational time to help researchers for development of medical devices. The results show that our parallel program can reduce the computation time by increasing the number of processors. Therefore, the parallel computing plays an important role in reducing the computational time. In order to obtain the better computational time, we can neglect NST and compute only the thrombus equation since the results are still reasonable. When high accurate result is required, we suggest that NST and the thrombus equation should be solved together. For the further work, we will develop the parallel computing algorithm to predict the formation of thrombus by changing flow pattern.

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