Parallel lattice-Boltzmann simulation of fluid flow in centrifugal elutriation chambers *

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Abstract. We present parallel lattice-Boltzmann simulations of fluid flow in a centrifugal elutriation chamber, a cell separation device for human blood cells. The critical factor in this separation technique is the hydrodynamic flow field. Understanding the influence of design parameters of a chamber on the flow field is important in optimizations of this process. Two different issues are considered in this paper: load balancing of the parallel lattice-Boltzmann simulations and preliminary simulations of fluid flow for a range of Reynolds numbers. It is shown that by exploiting appropriate load balancing strategies, such as the orthogonal recursive bisection method, the lattice-Boltzmann scheme is an efficient method for this application. Furthermore, 2D simulations confirm that the quality of separation degenerates above certain Reynolds numbers.

1 Introduction

Centrifugal elutriation is a physical cell separation technique by means of which differences in sedimentation velocity of human peripheral blood cells are exploited to isolate various types of cells [1–4]. The core of this technique is the combined effect of centrifugal and hydrodynamic forces acting on blood cells which are moving in a rotating chamber. The geometry of the separation chamber is a critical factor and therefore simulation of flow in this particular geometry can provide insights in optimization of this technique. We have applied the lattice-Boltzmann method to simulate this application, because of its suitability for a large range of complex geometries. Also, the effect of the cell load on the flow field can, in principle, be studied in the framework of the lattice-Boltzmann method.

The lattice-Boltzmann method [5,6] is a relatively new tool in computational fluid dynamics. It originated from the lattice-gas model [7] and has a microscopic character, as opposed to the conventional approach based on a numerical solution

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of the Navier-Stokes equation [8]. The key idea behind the lattice-Boltzmann method is to model fluid flow by distributions of particles moving on a regular lattice. At each time step the particles propagate to a neighboring lattice point followed by local collisions in which their velocities are redistributed. This simulation method has proven to be successful in modeling and simulation of complex fluid dynamical problems for which the conventional macroscopic approach may be difficult to apply [9–12]. Another important advantage of the lattice-Boltzmann method is the inherent spatial locality of the updating rules. This property makes it ideal for parallel processing.

The geometry of the elutriation chamber is in principle a tube of varying cross-section. Standard decomposition of the computational grid in equal sub volumes [13–15], which is a traditional parallelization approach in many lattice-Boltzmann simulations, will now be inefficient due to the inhomogeneity of the geometry. Therefore, an important issue for efficient parallel simulation of this application is load balancing.

In this article we first briefly introduce the lattice-Boltzmann method and discuss the centrifugal elutriation process. Then we shall discuss in detail the load balancing strategies and finally preliminary simulations will be presented.

2 The centrifugal elutriation technique

Since 1948 centrifugal elutriation has been available as a cell separation technique [4]. This technique is used to separate similar but slightly different cells as well as to obtain valuable information on size and mass. It has been used comparatively little until the mid-seventies, since available systems have been complex and lacking sensitivity. These difficulties have been overcome nowadays using simple design principles and this separation technique is promising because it does not effect the metabolism of the cell culture.

In centrifugal elutriation a fluid is pumped into a divergent chamber which is rotating and re-converges into a small outlet tube. A cell suspension is injected into the rotor and moves through the system into the separation chamber (see Fig. 1).

To gain insight in the centrifugal elutriation principle, we derive in this section a simple $1D$ model for the motion of a cell. In this model we assume that cells are spherical, the flow is laminar, the interactions between the cells are ignored and the Coriolis force and gravity are neglected [1].

The acceleration of a cell in the rotor chamber is determined by the imbalance of the drag and the centrifugal force. For a certain cell the drag force depends on the hydrodynamic velocity field, while the centrifugal force depends on the angular velocity and the radial distance. The hydrodynamic velocity in the separation chamber is assumed to scale inversely proportional with the cross-section of the chamber,

$$v = \frac{q}{A(r)} + \frac{dr}{dt} \tag{1}$$

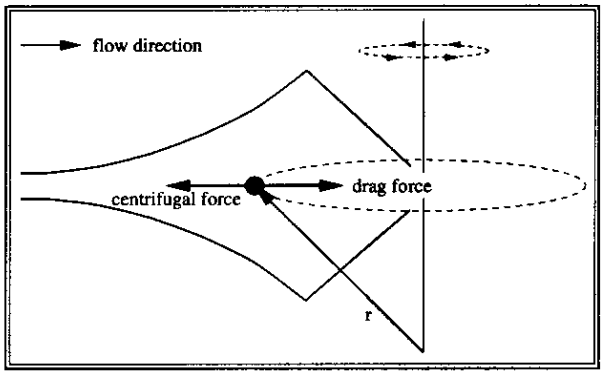


Fig. 1. A side-view of the centrifugal elutriation chamber. The centrifugal and the drag force are acting in opposite directions.

where q is the volumetric flow rate of the separating fluid, A the cross-sectional flow area which depends on r, the radial distance from the center of the rotor.

Within these assumptions, the motion of a blood cell is governed by the following equation,

$$\frac{d^2r}{dt^2} = \frac{\rho_c - \rho_f}{\rho_c}\omega^2 r - \frac{18\nu}{\rho_c d^2}\left(\frac{q}{A(r)} + \frac{dr}{dt}\right) \tag{2}$$

where ρ_c is the density of the cell, ρ_f the density of the fluid, ω the angular velocity, ν the viscosity of the fluid, q the volumetric flow rate of the separating fluid, t the time and d the diameter of the cell. The special design of the separation chamber coerces the cells to rest, relative to the rotor, at a point where the outward directed centrifugal forces (first term in Eq. 2) are balanced by the inward directed fluid dynamics (second term in Eq. 2). Such a steady state condition, established for cells at rest, relative to the rotor, at a distance r, is approximated by [1]:

$$r = \frac{18\nu q}{(\rho_c - \rho_f)\omega^2 d^2 A(r)}. \tag{3}$$

In summary, we see that according to this simple model the quality of the separation technique is mainly determined by the shape of the chamber. The implicit assumption in this model is that the hydrodynamic velocity field is uniform on planes perpendicular to the radial axes *and* the magnitude of the velocity is scaling inversely proportional with the cross-sectional area of the chamber. In the last section we will verify this assumption by studying the flow profiles. The effect of increasing the Reynolds number on the scaling of the velocity profile along the chamber will be also investigated.

3 The lattice-Boltzmann method

In lattice-Boltzmann methods particles move synchronously along the bonds of a regular lattice, and interact locally according to a given set of rules. Basically this method consists of the following two phases.

1. Propagation; in this phase particles move along lattice bonds to the neighboring lattice nodes.
2. Collision; particles on the same lattice node shuffle their velocities locally such that mass and momentum are conserved.

During the past years a variety of lattice-Boltzmann models have been developed. The differences lie e.g. in the connectivity of the lattice being used and the exact formulation of the collision operator [5,6]. The simplest one among these models is the so-called lattice-BGK (Bhatnagar-Gross-Krook) model where the collision operator is based on a single time relaxation to the local equilibrium distribution [16]. For two-dimensional simulations the D_2Q_9 (D is the number of dimensions and Q denotes the number of lattice bonds) is regularly used. Here each lattice point is connected with its eight nearest and diagonal neighbors. A rest particle is also included in order to improve the physical behavior and the stability of the method. The dynamics of the lattice-BGK model is given by the equation [16],

$$f_i(\mathbf{r}+\mathbf{c}_i, t+1) = f_i(\mathbf{r},t) + \frac{1}{\tau}(f_i^{(0)}(\mathbf{r},t) - f_i(\mathbf{r},t)) \quad , \tag{4}$$

where $\mathbf{c}_i$ is the i-th link, $f_i(\mathbf{r},t)$ is the density of particles moving in the $\mathbf{c}_i$-direction, τ is the BGK relaxation parameter, and $f_i^0(\mathbf{r},t)$ is the equilibrium distribution function towards which the particle populations are relaxed. The hydrodynamic fields such as the density (ρ) and the velocity ($\mathbf{v}$) are obtained from moments of the discrete velocity distribution $f_i(\mathbf{r},t)$ as

$$\rho(\mathbf{r},t) = \sum_{i=0}^{8} f_i(\mathbf{r},t) \qquad \text{and} \qquad \mathbf{v}(\mathbf{r},t) = \frac{\sum_{i=0}^{8} f_i(\mathbf{r},t)\mathbf{c}_i}{\rho(\mathbf{r},t)}.$$

The equilibrium distribution function can be chosen in many ways. A common choice is [17]

$$f_i^0 = t_i\rho(1 + \frac{1}{c_s^2}(\mathbf{c}_i\cdot\mathbf{v}) + \frac{1}{2c_s^4}(\mathbf{c}_i\cdot\mathbf{v})^2 - \frac{1}{2c_s^2}v^2),$$

where t_i is a weight factor depending on the length of the link vector and c_s is the speed of sound. In the D_2Q_9 model, the weight factors can be chosen as $\frac{4}{9}$, $\frac{1}{9}$ and $\frac{1}{36}$ for the rest particle, nearest neighboring and diagonal neighboring links, respectively. It can be shown that these values yield to a correct hydrodynamic behavior for an incompressible fluid in the limit of low Mach and Knudsen numbers [17]. The speed of sound for this model and the kinematic viscosity of the simulated fluid in lattice units are $c_s = \frac{1}{\sqrt{3}}$ and $\nu = \frac{2\tau-1}{6}$, respectively [17].

4 Parallelization

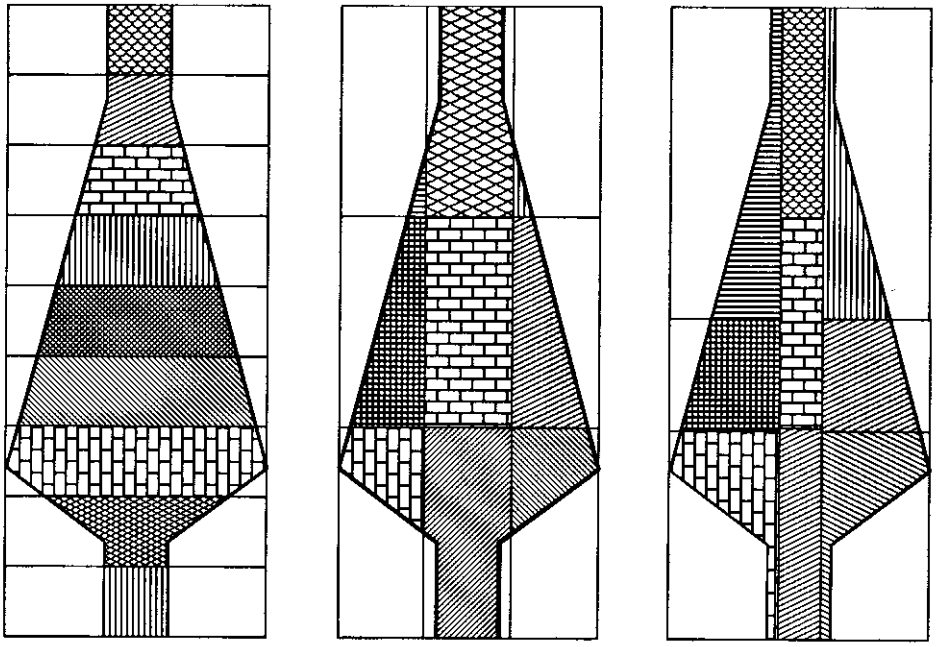
From test-simulations done on different lattice resolutions it became clear that large lattices (dimensions of 273×664) are required for our planned simulations (data not shown). The average error is then estimated to be around 3%. We have determined the error by comparing the hydrodynamic fields, like velocity and pressure, which were obtained on different lattice dimensions. Parallel computing is exploited here to facilitate efficient simulation of this problem. Basically parallelization of grid based algorithms like those of finite-difference, finite-element and lattice-Boltzmann models is done by means of the data decomposition strategy, where the computational grid is decomposed into sub-domains [18]. Each processor performs computations on a certain sub-domain and exchanges information with other nodes in order to resolve dependencies. The two factors controlling the efficiency of parallelization are the ratio between the communication time and the computation time, and the balance of workload among the processors. In Fig. 2.a and 2.b we show the decompositions which one would obtain if the problem was naively partitioned into equal sub volumes in one-dimension (slice decomposition) or two-dimensions (box decomposition). It is evident that the workload is not balanced in both cases (some processors get more computations to perform compared to the others) and thus more sophisticated load balancing is necessary for efficient parallel simulation of this problem.

The first step in load balancing is to find a partitioning of the grid such that differences in the workload of the processors are minimized. There are several ways to accomplish this goal, namely

1. Orthogonal Recursive Bisection: the computational grid is decomposed into partitions in an orthogonal direction, such that the workload is balanced. On each partition the same procedure is applied recursively. Workload due to obstacles in the fluid is neglected (see Fig. 2.c);
2. the Recursive Spectral Bisection method [18]: in the Recursive Spectral Bisection method both the connectivity of the grid and the workload at each lattice point are taken into account to find partitions with an optimal balance of both communication and computation;
3. load balancing by means of optimization strategies [19]: in this strategy, the computation and communication times are modeled by means of a cost function, and a partitioning which minimizes this cost function is approximated by means of optimization methods like the Simulated Annealing or Genetic Algorithms.

We have chosen the ORB method for two reasons. First of all, from a practical point of view minimization of the computation time is more important than minimization of the communication time. It became evident from timing experiments that in the lattice-Boltzmann method the communication overhead is small for moderate lattice sizes. Secondly, the other two strategies are quite expensive and should be used when the communication time becomes significant.

The major difference between the ORB partitioning and the slice and box decompositions is the communication pattern of the processors. Each processor

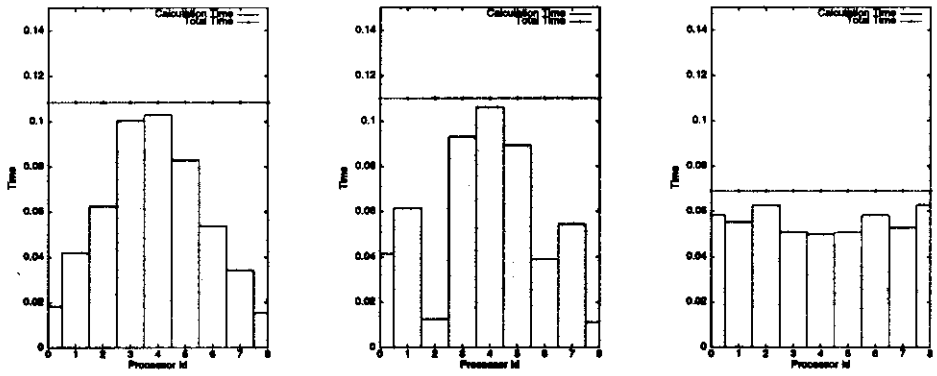


(a) Slice (b) Box (c) ORB

Fig. 2. Domain decomposition of a $2D$ model of the centrifugal elutriation chamber.

can now have a varying number of neighbors, and the interprocessor dependencies are more complicated for the corner points. This irregular communication pattern depends completely on the grid partitioning and thus on the geometry of the problem.

The calculation time per processor is shown in Fig. 2 for a run on 9 nodes. In this picture we have also included the cases when slice and box decomposition would have been applied to the same problem. It is evident that indeed both slice and box decomposition are inefficient approaches for this application. The workload between the processors is approximately balanced when the ORB method is used, while in slice and box decomposition big differences in the calculation times of the different processors are observed. The results of timing measurements for different number of processors are shown in Fig. 4. The ORB method is $10 - 60\%$ more efficient than the slice and box decomposition for a lattice of 139×332 points (for 32 processors the difference between the ORB and the other strategies becomes small, around 10%, because then the communication time is of the same order as the calculation time). We expect similar behavior when both the problem size and the number of processors are increased (the communication time scales as a surface while the calculation time scales as a



(a) Slice (b) Box (c) ORB

Fig. 3. Execution time per processor for the decompositions of Fig. 2

volume). The benefit gained by load balancing will certainly be significant for large-scale simulations (execution time of many hours) and even higher for complicated fluid-dynamical problems like simulation of particle - suspensions in a chamber.

5 Simulation results

In this section we will discuss some preliminary results of $2D$ simulations of fluid flow through the chamber. In these simulations the effect of the apparent forces due to rotation on the flow field is not taken into account. The flow boundaries are periodic along the radial direction and bounce-back [5] is used to model the solid walls. Periodic boundaries can only be used when the length of the inlet and the outlet tubes is long enough to guarantee that there is no interference between the values on the entrance and the exit of the chamber. A local body force is applied on each lattice point in order to drive the flow between the inlet and the outlet. The simulations have been performed on lattices of 273×664 and takes on the average around 30000 time-steps to reach steady state.

In Fig. 5 we show the flow profiles for different flow rates. We see that as the flow rate is increased the flow tends to become non-laminar. In principle the effective volume of the chamber is then reduced due to the vortices. In section 2 a one-dimensional model was discussed with the implicit assumptions that the velocity profile is uniform at faces which are perpendicular to the radial direction and that the magnitude of the velocity is scaling inversely proportional with the cross-sectional area of the chamber. We see that our $2D$ simulations suggest (see Fig. 5) that the flow profile is certainly not uniform at faces perpendicular to the radial axes.

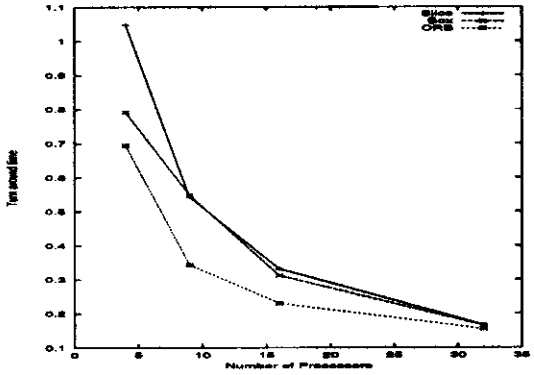
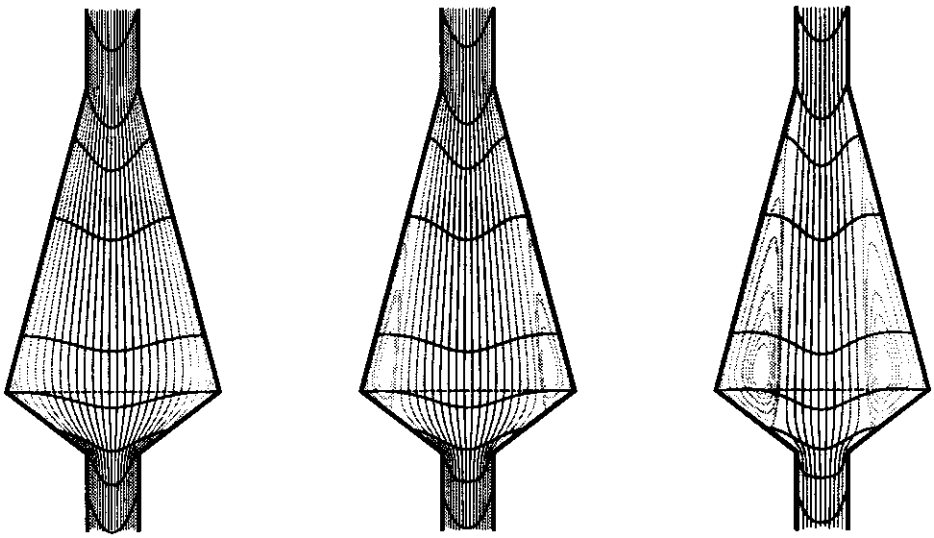


Fig. 4. The execution for different number of processors for slice, box and ORB decomposition



(a) Standard q. (b) 1.5 times q. (c) 3 times q.

Fig. 5. Velocity profile and streamlines at different volumetric flow rates q. The standard volumetric flow rate q is $3.029.10^{-7}$ (m^3/s). This corresponds at the entrance to a parabolic profile with a maximum velocity of 0.014 (m/s) in figure 5(a). The streamlines are grayscale colored with the norm of the velocity vector at that particular point. Darker lines correspond to a higher velocity of the fluid, lighter lines correspond to a lower velocity.

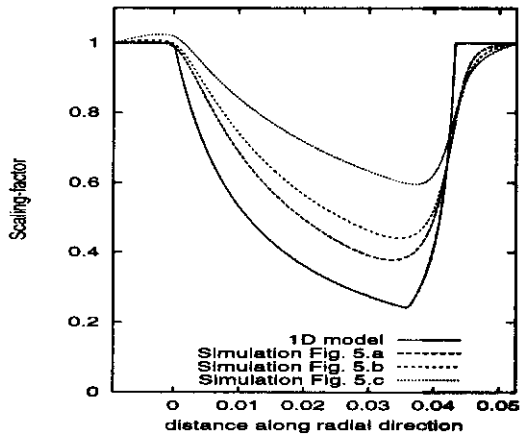


Fig. 6. The scaling factor for the simulations of Fig. 5 and the $1D$ model.

In principle the $1D$ model could still be useful when the velocity along the center line of the chamber would have a similar scaling behavior as Eq. 1 suggests. The scaling factor is now defined as the ratio between the magnitude of the velocity at a certain distance r along the center line, and the velocity at the entrance of the chamber. In Fig. 6 we have plotted this scaling factor along the chamber for the different Reynolds numbers which are shown in Fig. 5. We see that our simulated flow fields are not in agreement with the $1D$ assumption.

Our preliminary simulations suggest that more detailed simulations which include parameters like the chamber shape are necessary in order to understand the separation mechanism of the elutration technique. In future therefore $3D$ simulations will be performed in order to see whether the $1D$ model is adequate.

6 Conclusion and Future Work

In this paper we have discussed parallel lattice-Boltzmann simulations of fluid flow in centrifugal elutriation chambers. Two issues have been addressed, namely appropriate load balancing for efficient parallel simulation and the validity of an existing $1D$ model for the elutriation process. We found that by applying the Orthogonal Recursive Bisection method the workload is approximately balanced and thus good scalability results are obtained. Our $2D$ simulations are not in agreement with the $1D$ model. However $3D$ simulations are still required (since the effect of the walls is expected to be stronger then) in order to find out whether the $1D$ model is realistic. In future work we will also study the influence of different chamber shapes, inlet and outlet sections and flow-rates on the elutriation process. Our ultimate goal is to include transport of human blood cells in the chamber in order to study the effect of the cell load on the elutriation process.

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