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Parallel dilute particulate flow simulations in the human nasal cavity

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ABSTRACT

When simulating time-dependent particulate flows, one faces the dilemma that the domain decomposition used for fluid simulation is not optimal for parallel computation of particle trajectories. Therefore, the article proposes and compares two parallelization strategies for the particle phase based on the fixed domain decomposition approach used in the open source lattice Boltzmann framework OpenLB (http://www.openlb.net). The *communication optimal* strategy is found to be more efficient in the case of homogeneously distributed particles. Convergence studies and performance tests are conducted using a simplified geometry of the human lungs and show excellent parallel speedup. The implemented strategy is used to simulate time-dependent particulate flows of micro-particles in a patient-specific geometry of a human nasal cavity including paranasal sinuses. Dilute, uniformly distributed particles are released once at the start of inspiration, as well as repeatedly during the entire inspiratory cycle, which leads to a more homogeneous distribution. It is found that the deposition rates vary for the different injection methods.

1. Introduction

Airborne particulates pose a serious health risk. They may cause respiratory diseases such as lung cancer and asthma. On the other hand, purposefully used e.g. in nasal or asthma sprays they can help to treat such diseases. Investigating the deposition of particulates in the human respiratory system is therefore of great interest, however, *in vivo* examinations are risky, expensive and sometimes not feasible. Instead, simulations are feasible and provide detailed information on deposition. Yet, simulations of dilute particulate flows remain a challenging task in the research field of computational fluid dynamics (CFD). Especially transient flows through complex geometries such as the nasal cavity demand for computational power, that can only be satisfied by massive parallel systems. The Euler–Lagrange ansatz allows tracking of individual particles and is widely used to simulate such particulate flows. The Lattice Boltzmann method (LBM) is an explicit algorithm to compute fluid flows, that allows to embed a numerical integration scheme for particle tracking. One of LBM's greatest advantages compared to classical CFD methods is an efficient parallelization by domain decomposition [1–3]. Although parallelization of pure particle tracking is trivial, the coupling of both algorithms for transient flows poses a challenge. Computing particle trajectories on a different node as the respective fluid domain leads to high communication costs. Computation on the same node reduces parallel efficiency. In the scope of this article we tackle this dilemma by comparing two new parallelization strategies for the particle tracking algorithm based on the fixed domain decomposition of the fluid. The less complex strategy is successfully used to simulate time-dependent particulate flows in the human respiratory system.

Flow characteristics in the human airways have been studied before, both experimentally and numerically. In a general manner, Kleinstreuer and Zhang [4] provide a detailed overview on publications considering state-of-the-art models, experimental observations and computer simulations for all parts of the respiratory system. Vasconcelos et al. [5] simulated impact distributions of particles in a model of the tracheobronchial tree and stated a simple connection between the Stokes number and the escape rate. Studies concerning the particle deposition in the human nasal cavity have been performed in the past, experimentally on nasal airway replicas (Cheng et al. [6]; Kelly et al. [7]) as well as *in vivo* measurement on humans (Cheng et al. [8]). Finck [9] simulated particulate flows through the model of a nasal cavity using LBM and Lagrangian particle tracking. Usually in numerical studies particles are injected only once at a certain time, e.g. to model particle drug delivery with a nasal spray (Chen et al. [10]; Inthavong et al. [11,12]). In most of the studies, a constant inhalation flow rate with constant inlet velocity at the nostrils is used, while simulations of unsteady inhalation are rare in literature. To our knowledge only Se et al. [13] simulated particle deposition with an unsteady flow. When simulating flow in nasal cavities most authors

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omit the paranasal sinuses. As far as known to the authors, only Tu et al. [14] investigated deposition of nanoparticles for laminar flow in a geometry considering sinuses with focus on the diffusion process.

The objective of this article is to provide a parallel algorithm to simulate unsteady particulate flows in the human respiratory system. It is organized as follows: In Section 2, the mathematical modeling and numerical methods for particulate flows are introduced. In Section 3 two new parallelization strategies are proposed and compared concerning their respective computational and communication complexity. Section 4 presents numeric results for the more efficient algorithm. It is validated and speedup tests are performed. It is then used to simulate unsteady particle laden flows in the complex geometry of a patient specific nasal cavity including paranasal sinuses.

2. Material and methods

2.1. Mathematical modeling

To simulate the dynamics of disperse two-phase flows two different possibilities are standard: firstly, the Euler–Euler and secondly, the Euler–Lagrangian approach. The first one considers the continuous as well as the disperse phase to be homogeneous and uses Eulerian representation for both. In the second approach only the fluid phase has an Eulerian representation, while for each particle of the discrete phase the trajectory is tracked individually in a Lagrangian way. For particles with diameter $d_P > 1$ μm usually the Euler–Lagrange modeling approach is used. In particular, the fluid phase is not influenced by the particles (one way coupling). For smaller particles ($1 < d_P < 150$ nm) usually the Euler–Euler approach is employed. In finding particle deposition patterns in the human respiratory system the continuous phase is air. We choose to approximate it as an incompressible Newtonian fluid, which is the general approach for flows with Mach number less than 0.3. Therefore the incompressible Navier–Stokes equations apply

$$\begin{aligned} \frac{\partial \boldsymbol{u}_\mathrm{F}}{\partial t} + (\boldsymbol{u}_\mathrm{F}\cdot\nabla)\boldsymbol{u}_\mathrm{F} &= -\frac{1}{\rho}\nabla p + \nu\Delta\boldsymbol{u}_\mathrm{F} && \text{in } (t_0,t_1)\times\Omega, \\ \nabla\cdot\boldsymbol{u}_\mathrm{F} &= 0 && \text{in } (t_0,t_1)\times\Omega, \end{aligned} \tag{1}$$

where $p : (t_0,t_1)\times\Omega \to \mathbb{R}$ denotes the pressure and $\boldsymbol{u}_\mathrm{F} : (t_0,t_1)\times\Omega \to \mathbb{R}^3$ the fluid velocity, where $\Omega \subseteq \mathbb{R}^3$ represents the domain, $(t_0,t_1) \subseteq \mathbb{R}$ the considered time interval, ν the kinematic viscosity and ρ the fluid density.

Each particle of the disperse phase is tracked according to Newton's second law of motion

$$m_\mathrm{P}\frac{\partial \boldsymbol{u}_\mathrm{P}}{\partial t} = \boldsymbol{F}_\mathrm{P} \quad \text{in } (t_0,t_1)\times\Omega.$$

We assume particles to have velocity $\boldsymbol{u}_\mathrm{P} : (t_0,t_1) \to \mathbb{R}^3$ and constant mass $m_\mathrm{P} \in \mathbb{R}_{>0}$. The force $\boldsymbol{F}_\mathrm{P} = \sum_i \boldsymbol{F}_{\mathrm{P},i}$ can be composed of forces $\boldsymbol{F}_{\mathrm{P},i}$ acting on the particles, such as Stokes drag force $\boldsymbol{F}_\mathrm{St} = 6\pi a\mu_\mathrm{F}(\boldsymbol{u}_\mathrm{F} - \boldsymbol{u}_\mathrm{P})$. Other forces, such as Basset force or virtual mass are extremely small in the considered setup and can be neglected [15].

2.2. Discretization

In the following the introduced equations are discretized according to the used numerical methods.

2.2.1. Fluid phase (Euler)

The considered subclass of LBMs enables the simulation of the dynamics of incompressible Newtonian fluids. Instead of directly computing the quantities of interest, which are the fluid velocity $\boldsymbol{u}_\mathrm{F} = \boldsymbol{u}_\mathrm{F}(t,\boldsymbol{r})$ and fluid pressure $p = p(t,\boldsymbol{r})$ for $\boldsymbol{r} \in \Omega$ and $t \in [t_0, t_1]$, a lattice Boltzmann numerical model computes the dynamics of particle distribution functions $f : [t_0,t_1]\times\Omega\times\mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ in a phase space $\Omega\times\mathbb{R}^3$ with position $\boldsymbol{r} \in \Omega$ and particle velocity $\boldsymbol{v} \in \mathbb{R}^3$. The continuous transient phase space is replaced by a discrete position space Ω_h with a spacing of $\Delta\boldsymbol{r} = h$ for the positions, a set of $q \in \mathbb{N}$ vectors $\boldsymbol{v}_i$ for the velocities and a spacing of $\Delta t = h^2$ for time. The resulting discrete phase space is called the *lattice* and is labeled with the term *DdQq*. To reflect the discretization of the velocity space, the continuous distribution function f is replaced by a set of q distribution functions $f_i : [t_0,t_1]\times\Omega \to \mathbb{R}_{\geq 0}$ $(i = 0,1,\ldots,q-1)$, representing an average value of f in the vicinity of the velocity $\boldsymbol{v}_i$. Detailed derivations of various LBM can be found in the literature, e.g. in [16]. The iterative process in an LB algorithm can be written in two steps, the *collision step* (2) and the *streaming step* (3):

$$\widetilde{f}_i(t,\boldsymbol{r}) = f_i(t,\boldsymbol{r}) - \frac{1}{3\nu + 1/2}\left(f_i(t,\boldsymbol{r}) - M_i^\mathrm{eq}(t,\boldsymbol{r})\right), \tag{2}$$

$$f_i(t+h^2, \boldsymbol{r}+h^2\boldsymbol{v}_i) = \widetilde{f}_i(t,\boldsymbol{r}) \tag{3}$$

for $i = 0,1,\ldots,q-1$, where

$$M_i^\mathrm{eq}(t,\boldsymbol{r}) : = \frac{w_i}{w}\rho\left(1 + 3h^2\,\boldsymbol{v}_i\cdot\boldsymbol{u}_\mathrm{F}(t,\boldsymbol{r}) - \frac{3}{2}h^2\boldsymbol{u}_\mathrm{F}^2(t,\boldsymbol{r}) + \frac{9}{2}h^4(\boldsymbol{v}_i\cdot\boldsymbol{u}_\mathrm{F}(t,\boldsymbol{r}))^2\right)$$

is a discretized *Maxwell distribution* with moments ρ and $\boldsymbol{u}_\mathrm{F}$ given according to

$$\rho := \sum_{i=0}^{q-1} f_i \quad \text{and} \quad \rho\boldsymbol{u}_\mathrm{F} := \sum_{i=0}^{q-1} \boldsymbol{v}_i f_i.$$

The variable $\boldsymbol{u}_\mathrm{F}$ now denotes the discrete fluid velocity and ρ the discrete mass density given in Ω_h, which is related to the macroscopic pressure by $p = \frac{\rho}{3h^2}$. The kinematic fluid viscosity ν is assumed to be given, and the terms w_i/w, $\boldsymbol{v}_i h$ $(i = 0,1,\ldots,q-1)$ are constants depending on the LBM of choice. The discrete fluid velocity $\boldsymbol{u}_\mathrm{F}$ and the discrete pressure p can be related to the solution of a macroscopic initial value problem, governed by an incompressible Navier–Stokes equation, as shown in [17].

2.2.2. Particle phase (Lagrange)

If the fluid velocity at position $\boldsymbol{r} \in \Omega$ of a particle is known, it is possible to compute the particle velocity by solving

$$m_\mathrm{P}\frac{\partial \boldsymbol{u}_\mathrm{P}}{\partial t} = \boldsymbol{F}_\mathrm{St},$$

where $\boldsymbol{F}_\mathrm{St} = \boldsymbol{F}_\mathrm{St}(t,\boldsymbol{u}_\mathrm{P}(t)) = 6\pi a\mu_\mathrm{F}(\boldsymbol{u}_\mathrm{F}(t) - \boldsymbol{u}_\mathrm{P}(t))$ is Stokes' drag force. The backward Euler method with the following update rule

$$\boldsymbol{u}_\mathrm{P}(t+kh^2) = \boldsymbol{u}_\mathrm{P}(t) + \frac{kh^2}{m_\mathrm{P}}\,\boldsymbol{F}_\mathrm{St}(t+kh^2, \boldsymbol{u}_\mathrm{P}(t+kh^2))$$

is used, with the initial condition $\boldsymbol{u}_\mathrm{P}(t_0) = \boldsymbol{u}_\mathrm{F}(t_0)$ and a small $k \in \mathbb{N}$. This does not lead to an implicit non-linear system of equations, since substituting

$$\boldsymbol{F}_\mathrm{St}(t+kh^2, \boldsymbol{u}_\mathrm{P}(t+kh^2)) = 6\pi a\mu_\mathrm{F}\left(\boldsymbol{u}_\mathrm{F}(t+kh^2) - \boldsymbol{u}_\mathrm{P}(t+kh^2)\right)$$

in the last equation, leads to

$$\boldsymbol{u}_\mathrm{P}(t+kh^2) = \boldsymbol{u}_\mathrm{P}(t) + kh^2\sigma\left(\boldsymbol{u}_\mathrm{F}(t+kh^2) - \boldsymbol{u}_\mathrm{P}(t+kh^2)\right),$$

with $\sigma = \frac{6\pi a\mu_\mathrm{F}}{m_\mathrm{P}}$. Rearranging leads to

$$\boldsymbol{u}_\mathrm{P}(t+kh^2) = \frac{\boldsymbol{u}_\mathrm{P}(t) + kh^2\sigma\,\boldsymbol{u}_\mathrm{F}(t+kh^2)}{1+kh^2\sigma}.$$

As $\boldsymbol{u}_\mathrm{F}$ is only available on lattice nodes, it is interpolated by a trilinear interpolation. Therefore lattice refinement can influence the particle trajectories.