LBM SIMULATION OF THE PARTICLE DEPOSITION IN THE CHILDREN AIRWAYS WITH THE USE OF OPENLB

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Abstract

Aerosol particles like dust involved in the air can pass through the respiratory tract and can be deposited there. The long-term deposition of fine solid particles in the lower airways can stimulate lung diseases. In contrary, for the healing of certain lung diseases, the delivering of medicament's to the lower airways is important. Computational Fluid Dynamics (CFD) enables to simulate the flow field and the particles deposition in the lungs. By this method, it is possible to identify the probability of reaching particles into the lower airways through the tracheo-bronchial tree. In this poster, the flow field in the child lungs (5-year-old) in a constant sedentary breathing regime was simulated using the Lattice Boltzmann Method (LBM) with the LES Smagorinsky turbulence model. To verify the calculated velocities by LBM in OpenLB software, the finite volume LES Wale simulation in Star-CCM+ was performed. The results showed a good agreement of the fluid flow, some discrepancies were found for deposition of particles. Nevertheless, LBM and OpenLB were proven to be a capable tool to solve the air flow through the respiratory tract is possible to use for particle deposition.

1. Introduction

Project motivation: support experimental work on our institute by LBM method. Till now the FVM and usage of Star-CCM+ was only tool to support experimental work on our department. Comparison of different numerical methods and experimental work is important for fundamental research of aerosol deposition in the human lungs (adult, children) .

Lattice Boltzmann Method (LBM): Mesoscopic numerical method based on the statistical molecular dynamics described by the Boltzmann equation with the distribution function $f(\vec{x},\vec{\xi},t)$ used for fluid flow simulation.
Velocity discretization: Velocity set D3Q19.
Time and spatial discretization: fully discretised Boltzmann equation with the BGK collision operator:

$$f_i(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = f_i(\vec{x},t) - \frac{\Delta t}{\tau}\left[f_i(\vec{x},t) - f_i^{eq}(\vec{x},t)\right]$$

Macroscopic quantities: given by the moments of the distribution function $f(\vec{x},\vec{\xi},t)$:

$$\rho(\vec{x},t) = \int f(\vec{x},\vec{\xi},t)d^3\xi$$
$$\rho(\vec{x},t)\,\vec{u}(\vec{x},t) = \int \vec{\xi} f(\vec{x},\vec{\xi},t)d^3\xi$$
$$\rho(\vec{x},t)E(\vec{x},t) = \int |\vec{\xi}|^2 f(\vec{x},\vec{\xi},t)d^3\xi$$

Particle simulation: particles are solved by Lagrangian multiphase particles model using drag coefficient C_D by Schiller-Neumann, the same model is also used in Star-CCM+.

2. Simulation setup

We simulated constant inspiration in a sedentary regime of 10.5 l/min with inhalation of aerosol particles to bronchial tree by suction. Velocity inlets are at the bottom of lungs and have negative velocities. The pressure outlet is on the entrance to the inhalator mask. Geometry was produced by rescaling of adult human airways to the 2[nd] bifurcation.

FVM simulation: steady inhalation by unsteady solver LES Wale (C_w =0.544, C_t =3.5, κ = 0.41). It is Wall-Adapting Local-Eddy viscosity model setup by default settings in software Star-CCM+. The used base size of FVM cells was $5 \cdot 10^{-4}$ m and $1.14 \cdot 10^{-5}$ m in prismatic layer near wall vicinity. Time step was $5 \cdot 10^{-5}$ s. The simulated time was 10 s (2 s stabilization + 8 s averaging including particles). Particles are solved by Lagrangian multiphase model.

LBM LES Smagorinsky subgrid-scale model: eddies smaller than defined grid length modelled by adding artificial turbulent viscosity v_{turb} to the model with default Smagorinsky constant $C_f = 0.1$. Velocity set D3Q19. We used BGKSmaogrinskyDynamics and Bouzidi wall bc. The simulated time was 1.5 s (ramp 0.1 s + stabilization 0.4 s + 1 s averaging including particles).

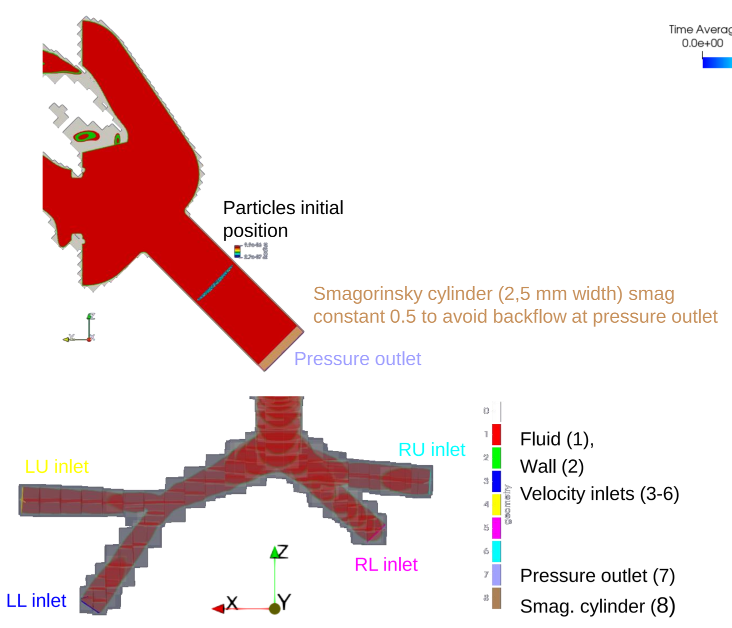
Velocity inlets (piston profiles)	
Left inlets	**Right inlets**
v_LU = -3.3 m/s (Re = 990)	v_RU = -2.7 m/s (Re = 810)
v_LL = -2.7 m/s (Re = 810)	v_RL = -4.3 m/s (Re = 1290)

Particles	
Count	300000
Radius min	$0.7\cdot10^{-7}$ m
Radius median	$2.5\cdot10^{-6}$ m
Radius max	$9.9\ 10^{-6}$ m
Density	998 kg/m³

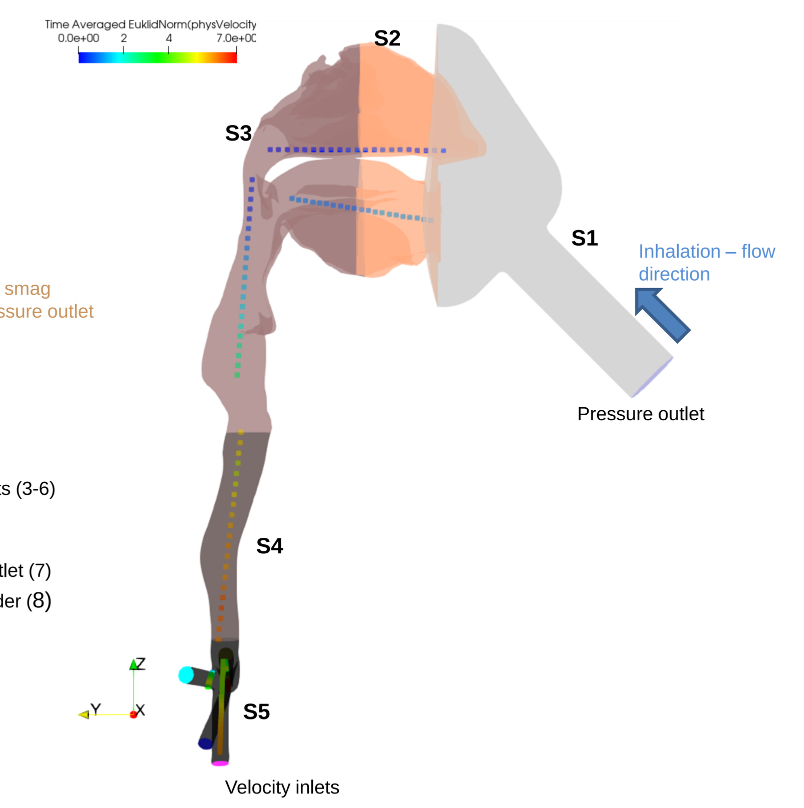
	3 cases with different refinement (N3000 used for validation of velocity field)			
	LBM_N	**2000**	**2500**	**3000**
	lattices	30 mil.	56 mil.	96 mil.
cell length	deltax [m]	$1.5\cdot10^{-4}$	$1.2\cdot10^{-4}$	$1\cdot10^{-4}$
time step	deltat [s]	$7.5\cdot10^{-7}$	$6\cdot10^{-7}$	$5\cdot10^{-7}$
relaxation time	tau	0.50185	0.502313	0.502775

3. Results

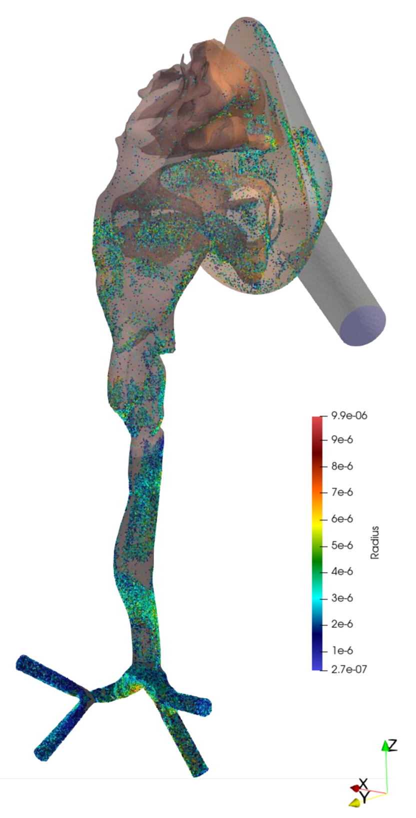
I. Geometry
Side slice with materials:



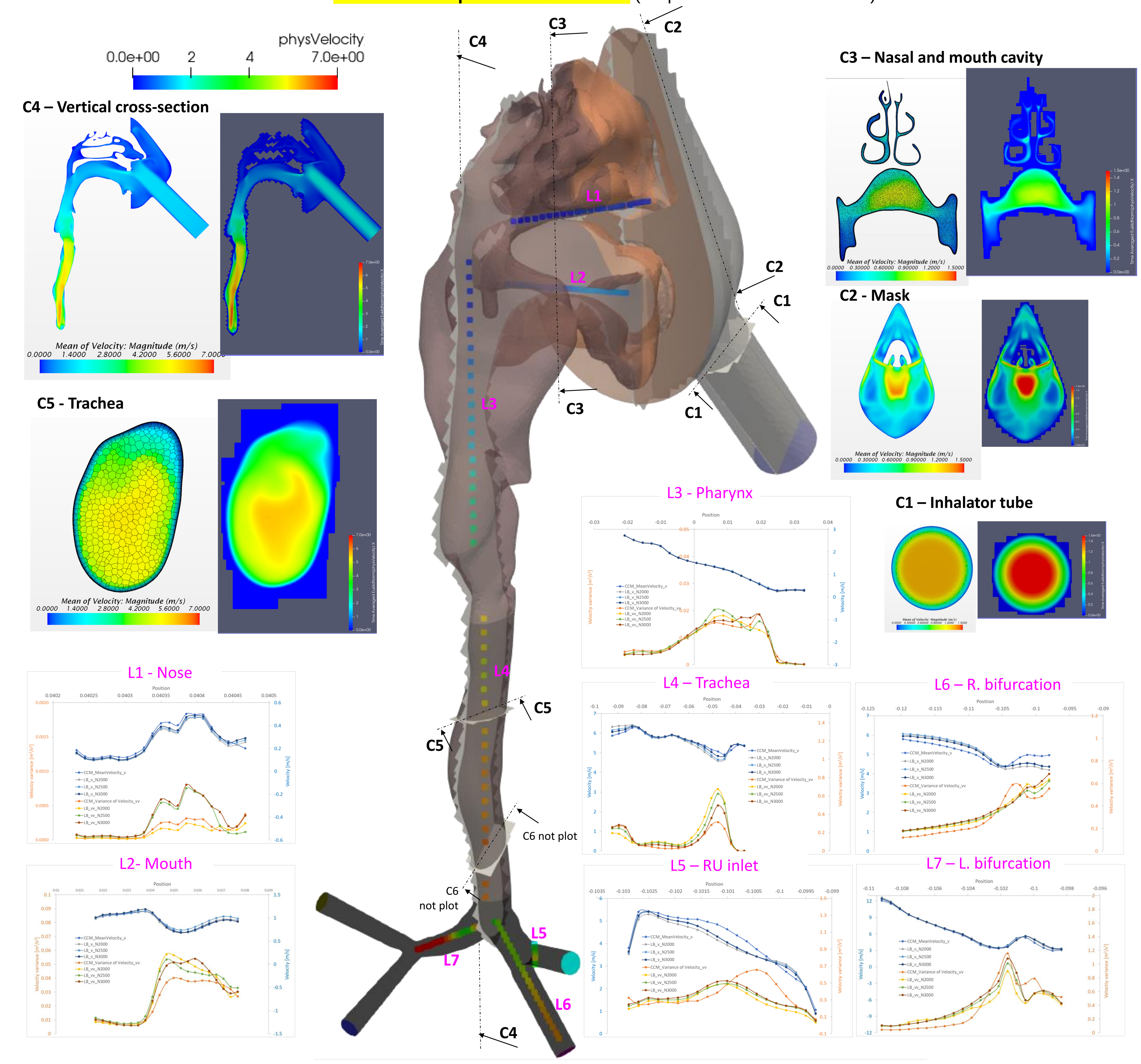
II. Velocities simulation (lineprobes)
Side view with velocity lineprobes and S1-S5 segments for which we have data about deposition.



III. Particles deposition
Visualisation of particle deposition with defined radius



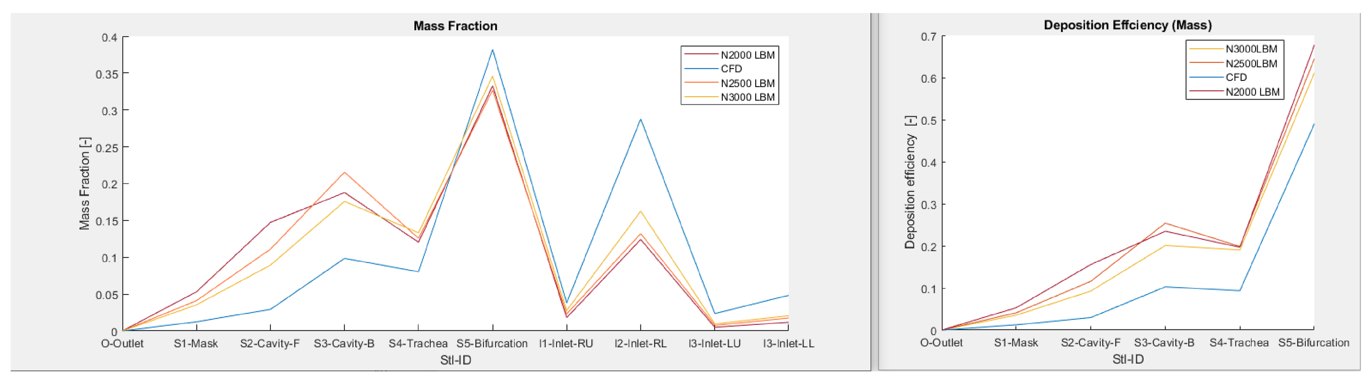
IV. Validation OpenLB vs Star-CCM+ (lineprobes and cross-sections)



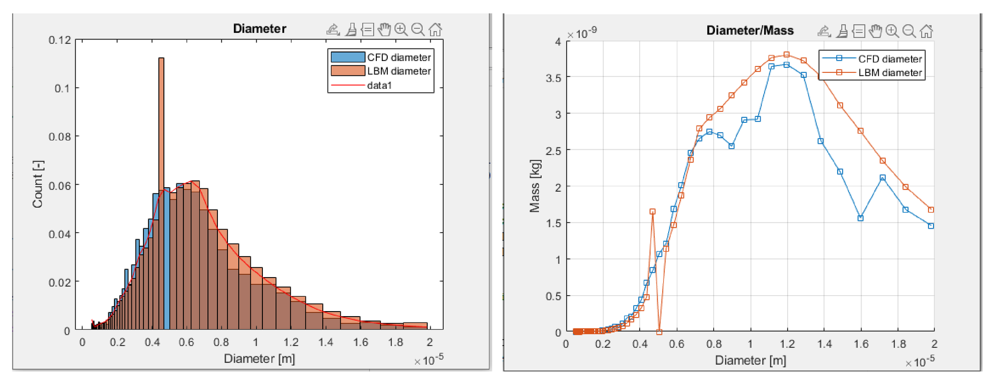
4. Discussion and issues

Simulation of velocity field is in LBM and FVM comparable. Differences in velocity magnitudes are negligible in the core of the flow. Slightly differences are at wall vicinity and also the velocity fluctuations differs.

The final results of **particle deposition** can be express by „Mass Fraction" and also „Deposition Efficiency". We have hypothesis that with increasing number of cells in OpenLB we are going closer to classical CFD software. But to get better results we suppose to deal with some issues.
On the figure below are the post-processed data about deposition. For this purposes we prepare the Matlab script for automatic evaluation based on the comparison closest distance of the non-active particles related to the local stl file, corresponding to the segments S1-S5 and all inlets and outlets..

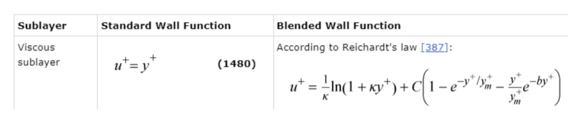


Our first idea what can be wrong was to compare the **particle size spectra** and mass distribution, see plots below. We found some small discrepancies, but no substantial. The difference in the spectra was caused by the coarser setup in OpenLB, when it uses step function instead of Star-CCM+ which interpolates the spectra by 100 particles bins based on probability function. We do not expect any significant influence on the deposition data caused by this problem.



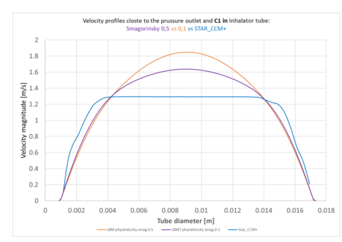
What **would be great to have** in OpenLB code implemented

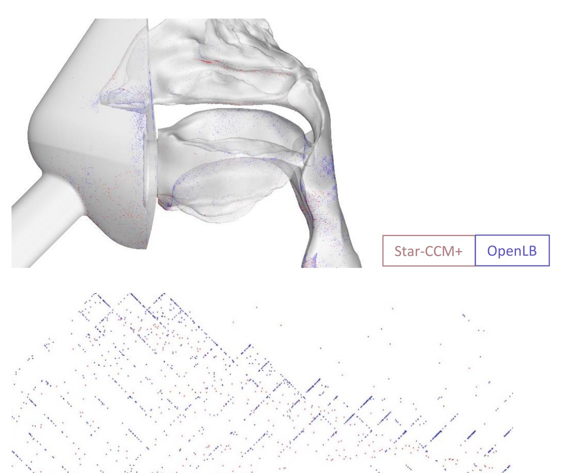
- Local refinement – local refinement can save cost for simulation processing (92 mil. Lattice versus 8 mil. FVM)
- Prismatic layers – even with such refinement which we did it is still significant difference between cell sizes due to the missing prismatic layer approach in OpenLB.
- Wall function – Star-CCM+ uses „All y+ wall treatment"



Other issues

- We observed in OpenLB the higher particles deposition in the mask especially on the face around the mouth and nose. From this reason we investigated the effect of Smagorinsky cylinder constant on the velocity profile close to the pressure outlet. The cylinder helps with stability during initialization and prevents to reverse flow in pressure boundary on pressure outlet





- Simulation of particle deposition with Bouzzidi has problem with stacking of the particles on the grid which forms structures on the wall of airways, which is in Star-CCM+ resolved by interpolation, however this fact has no big impact on the postprocessing of deposition.

5. Conclusion

We did simulation in OpenLB and Star-CCM+ on the 5yr_Mask lungs model. We compared the results of velocities field and also particle depositions. It can be concluded that OpenLB is able to resolve velocity field in such complex geometry (model includes nasal cavity) to obtain comparable results with Star-CCM+. In case of particle deposition we have some discrepancies, which we hope that can be solved by finer refinement. But it increases computational costs substantially. All results were recalculated on the current release of olb_1.5r0 from 14.4.2022.

The next step is to calculate cyclic breathing regime and other geometries. Also the simulated deposition data are planned to be validated by measurement in laboratory at Brno UT.

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