GPU parallelization of particle deposition in human lung airways

Lokesh Mohanty, Thivin Anandh, Sashikumaar Ganesan
STARS Lab

Motivation & Research Goals

Modeling particle deposition in human air pathways is important for understanding regional particle deposition which is crucial for targeted drug delivery. Studies have shown potential health risks associated with ultrafine particles deposited in lungs. Traditional techniques of in vivo and in vitro face significant challenges. And the commonly used Lagrangian approach is computationally intensive as it involves the tracking and interpolating of millions of particles at each time step. Due to the intricate nature of finite element method data structures, parallelizing the particle deposition on GPUs poses challenges.

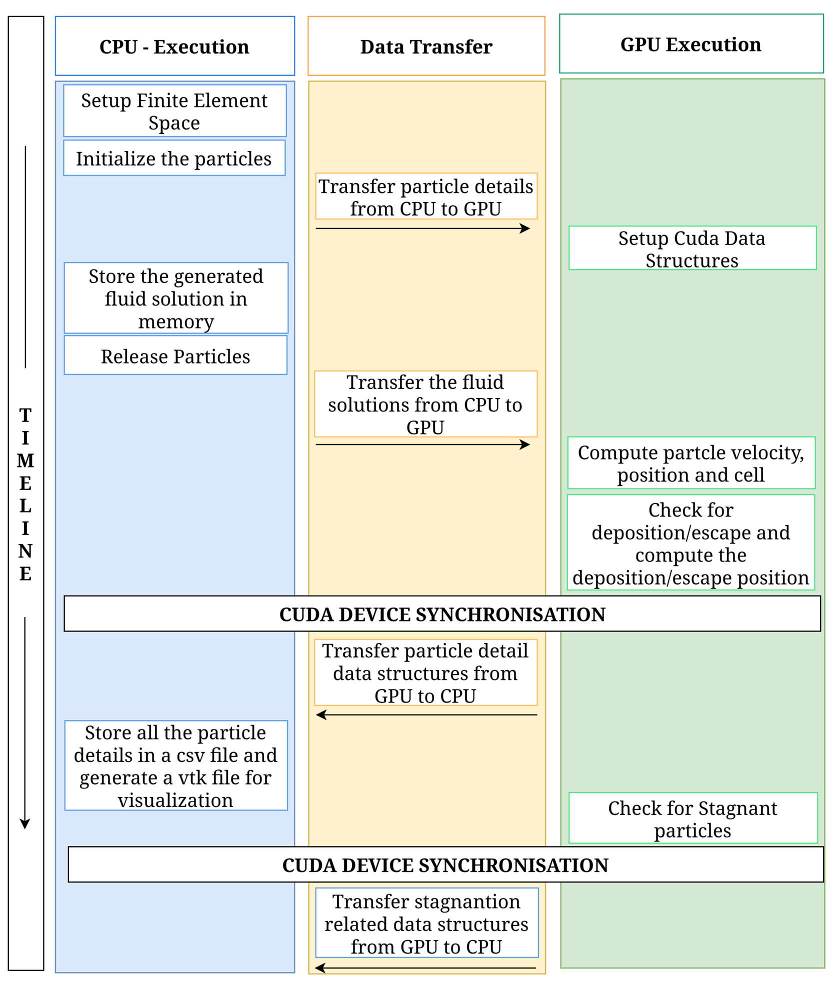
Methodology

Using ParMooN[1], an in-house FEM package, we solve the time dependent Navier-Stokes equation using variational multi-scale method. And using its results, the particles are simulated by a Lagrangian approach[2]. The equations of motion for the particles are given by

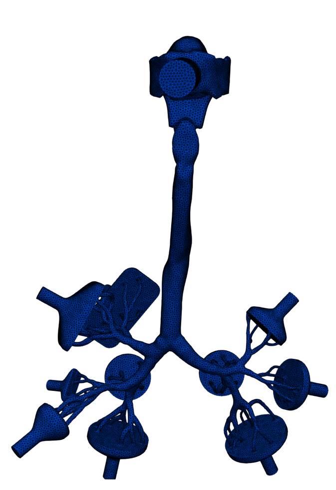
$$m_p \frac{d\mathbf{u}_p}{dt} = \frac{3}{4} \frac{\rho_f}{\rho_p} \frac{m_p}{d_p} \frac{C_D}{C_C} |\mathbf{u}_f - \mathbf{u}_p| (\mathbf{u}_f - \mathbf{u}_p) + m_p \mathbf{g} \frac{\rho_p - \rho_f}{\rho_p} + \mathbf{F}_B$$

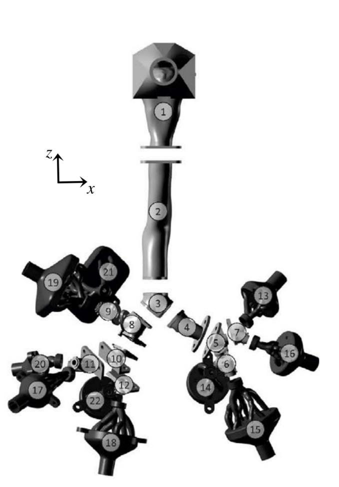
Here $\mathbf{u}_p$, $\mathbf{u}_f$, ρ_p, ρ_f, represents the particle velocity, fluid velocity, particle density and fluid density respectively. The terms in the right hand side are drag force, gravitational force and Brownian force respectively.

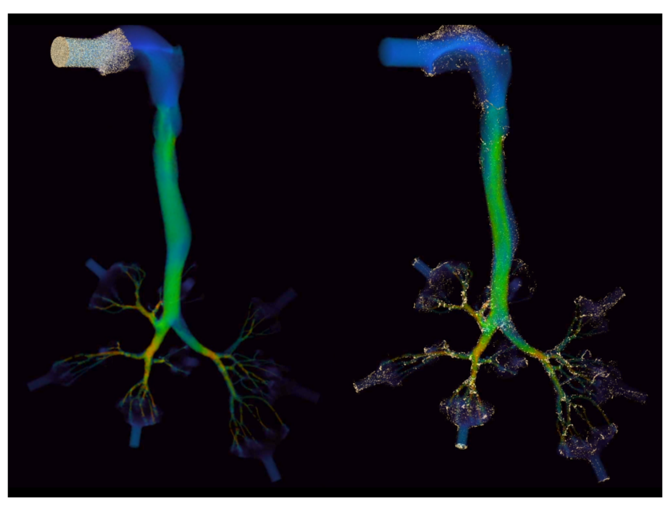
- The above equation is used to update the particle's current position at every time-step
- Based on the current position, the current cell is determined using a zonal-based search
- If the particle is outside the domain, based on the previous cell and current position, the deposition location is computed



- Mesh, Geometry (segmented), Begining of simulation, End of simulation

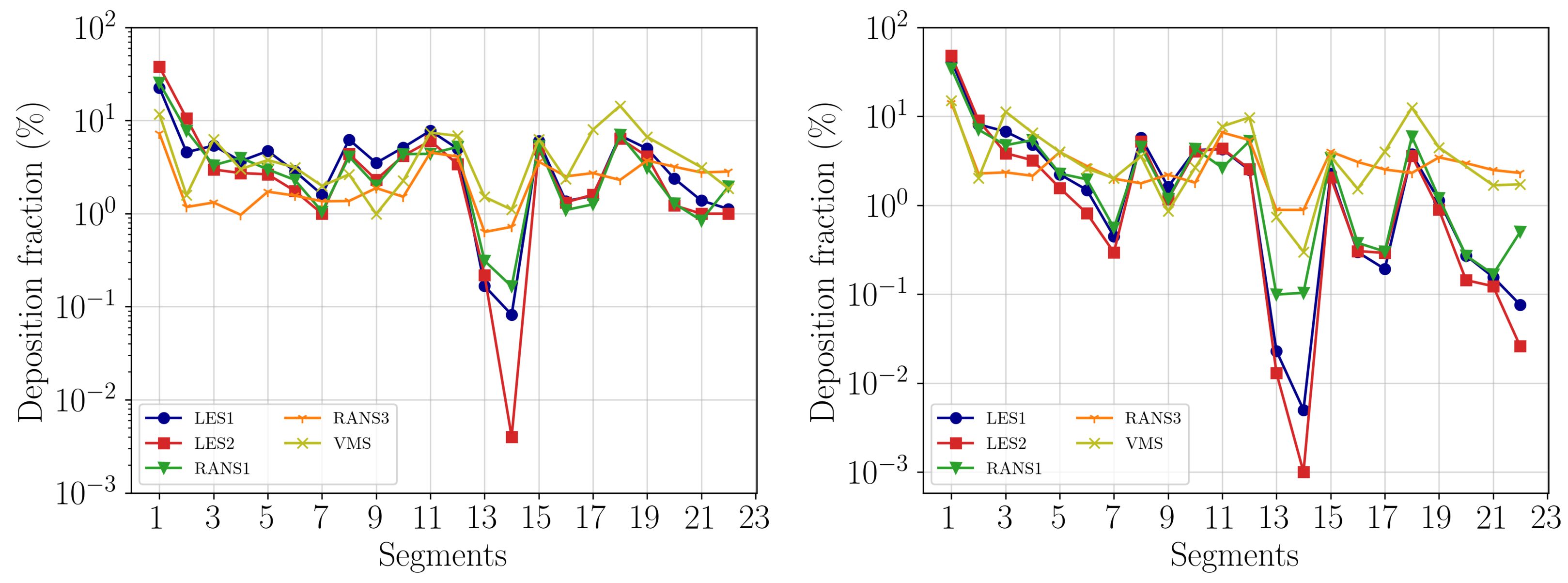




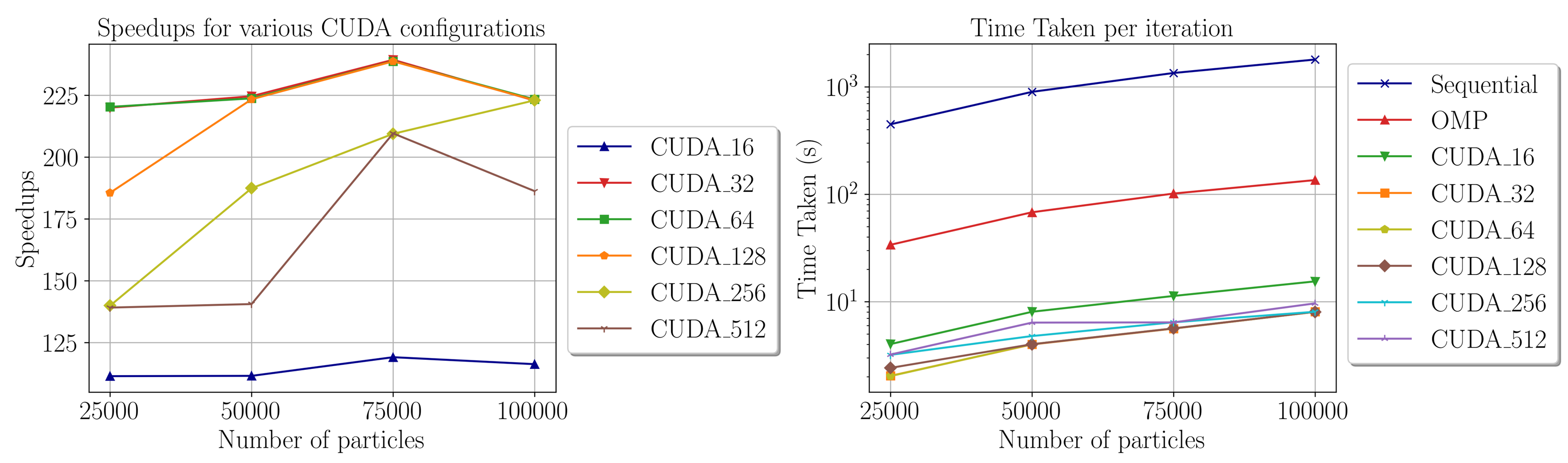


Results

- We validated the results of our model with existing literature[2] using deposition fraction at different segments of the lungs (8μm on left and 10μm on right).



- We achieved speedups of 13x for OpenMP and 220x for GPU when compared to the sequential.



Future Plan

- Integrate CUDA with MPI on a distributed computing setup to further improve the scalability of the particle tracking.
- Implement asynchronous data transfer within the GPU using CUDA streams to overlap the data-transfer with computation.

References

[1] ParMooN – a modernized program package based on mapped finite elements
U. Wilbrandt, C. Bartsch, N. Ahmed, N. Alia, F. Anker, L. Blank, A. Caiazzo, S. Ganesan, S. Giere, G. Matthies, R. Meesala, A. Shamim, J. Venkatesan, and V. John
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[2] Regional aerosol deposition in the human airways: The SimInhale benchmark case and a critical assessment of in silico methods.
P. Koullapis, S.C. Kassinos, J. Muela, C. Perez-Segarra, J. Rigola, O. Lehmkuhl, Y. Cui, M. Sommerfeld, J. Elcner, M. Jicha, I. Saveljic, N. Filipovic, F. Lizal, and L. Nicolaou
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