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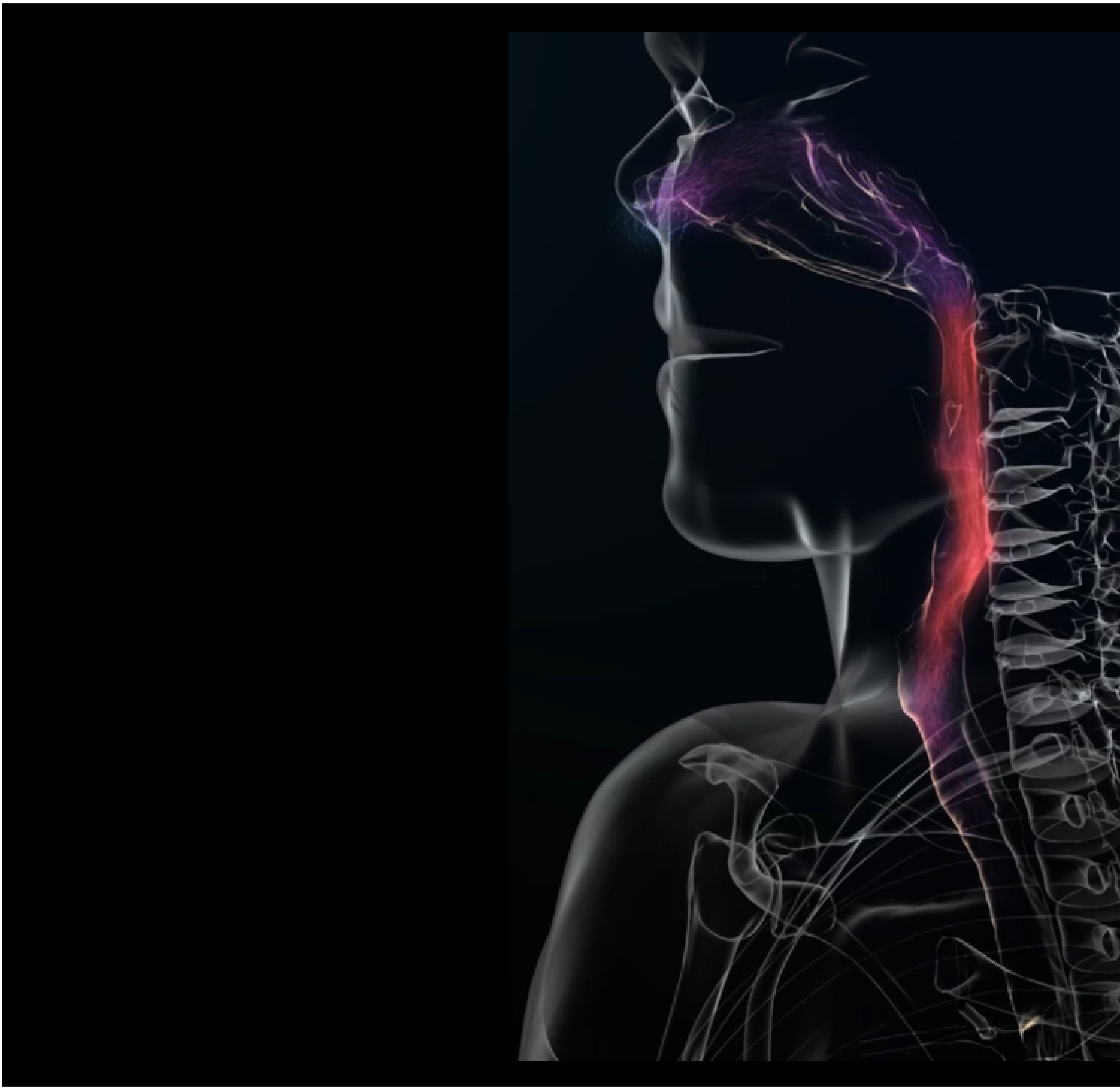
Respiratory system



The project aims at predicting particle deposition in the respiratoty system, drug delivery being the main target application. To this end, direct numerical simulation of the airflow and Lagrangian particle transport are carried out in the large and small airways.

Summary

The simulation of the respiratory system, and the transport of nano-particles through it, is of primary importance in the design of drug sprays. This research line consists in developing accurate numerical tools to predict patient specific flow dynamics and particle deposition if the large and small airways. This involves developing numerical techniques to accurately capture the coexisting laminar/transitional/tubrulent states of the flow, but also by developing robust numerical techniques specially designed for the transport of nano-particles (e.g. Brownian motion, adaptive time step).

From the computer science side, consequent work has been dedicated to the optimization of this coupled simulation. On the one hand, a single-code approach consists in solving the particle equations once the fluid solution has been obtained at the end of a time step, using the same instance of the same code. On the other hand, a multi- code approach enables one to overlap the transport of the particles with the next time step solution of the fluid equations, and thus obtain asynchronism. In this case, different codes or two instances of the same code can be used. Both approaches have been tested an compared. In addition, a dynamic load balancing library is used on the top of OpenMP pragmas in order to continuously exploit all the resources available at the node level, thus increasing the load balance and the efficiency of the parallelization.

Objectives

The objective of the research line is to investigate the physics of the inhalation process, from the nose, through the large airways, and down to the small airways. The study includes not only the simulation of the airflow but also the transport of particles and their depositions as they are advected towards the small airways. The main applications are drug spray design and toxicology, for which a comprehensive knowlegde of the particle paths is required.

The simulations of the unsteady flow dynamics are performed to resolve all the time and space scales, thanks to the use of massive computational resources. The highly parallel finite elements code Alya is used, for solving the transient incompressible Navier-Stokes equations on unstructured meshes. Particle transport is carried out asynchronously, in run time, using a second instance of Alya. Together with a dynamic load balancing, this technique enables the transport of millions of particles while resolving the fluid equations at the same time.

The research is done in collaboration with the Imperial College and Saint Mary's hospital in London, and with the computer Science Department of BSC.

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