SUCCESS STORY

Leveraging cloud resources to optimise drug delivery to lungs

Drug delivery through simulations on a realistic dosage

Estimates suggest that 20 million people have been diagnosed with asthma, 2.5 million with chronic obstructive pulmonary disease (COPD), and over 250,000 with interstitial lung diseases in Europe and the UK.

Patient-specific computer-aided simulations of aerosol inhalation can be a viable approach to optimise drug delivery to the lungs. Our research uses patient-specific medical images (computed tomography (CT) scans of lungs) to construct lung airways and multi-scale computational particle-fluid dynamics (CPFD) to simulate transport and deposition of aerosol drug particles in the airways.

Our ultimate goal is to provide clinicians with tailored treatment recommendations and underpin decisions in precision respiratory medicine. We also aim to educate patients on inhaler techniques through visualisations of drug deposition in their own airways.

Similar studies exist but, unfortunately, they've been conducted with a significantly smaller number of particles which do not correspond to the realistic inhaler dose. This limitation is related to the significant computational resources needed to perform such simulations.

We seek to evaluate the implications of underestimating the drug concentration by being the first research group to perform simulations on a realistic dosage being inhaled by a patient. To date, simulations of this size couldn't be achieved, but we intend to demonstrate that they can be deployed feasibly thanks to powerful cloud computing services.

> “Physiologically accurate models with realistic dosage provide high-fidelity flow physics, but the complexity of the lung creates demanding and long simulations due to huge computational power and time requirements.

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FIELD OF STUDY
Medical & Health Sciences

LOCATION
United Kingdom

OCRE RESOURCES USED
Cloud Service

CHALLENGE

Accurate prediction requires high computational expense

Computational particle-fluid dynamics, an in silico method, can incorporate the multiscale physics of airflow and aerosol deposition in lungs. In existing models, the number of drug particles or droplets is significantly smaller than that of realistic dosages released from the inhaler due to high computational expense. This reduction (typically by a factor of 105) leads to poor prediction of forces acting on aerosols, turbulence-aerosol, and boundary-aerosol interactions. In comparison to a true inhaler, where there are billions of particles with a size distribution, transport phenomena are significantly altered due to higher local particle concentration. Oversimplification could lead to poor predictions of drug deposition and misinformed treatments for patients. Physiologically accurate models with realistic dosage provide high-fidelity flow physics, but the complexity of the lung creates demanding and long simulations due to huge computational power and time requirements. These simulations have now been feasible with cloud high performance computing configurations.

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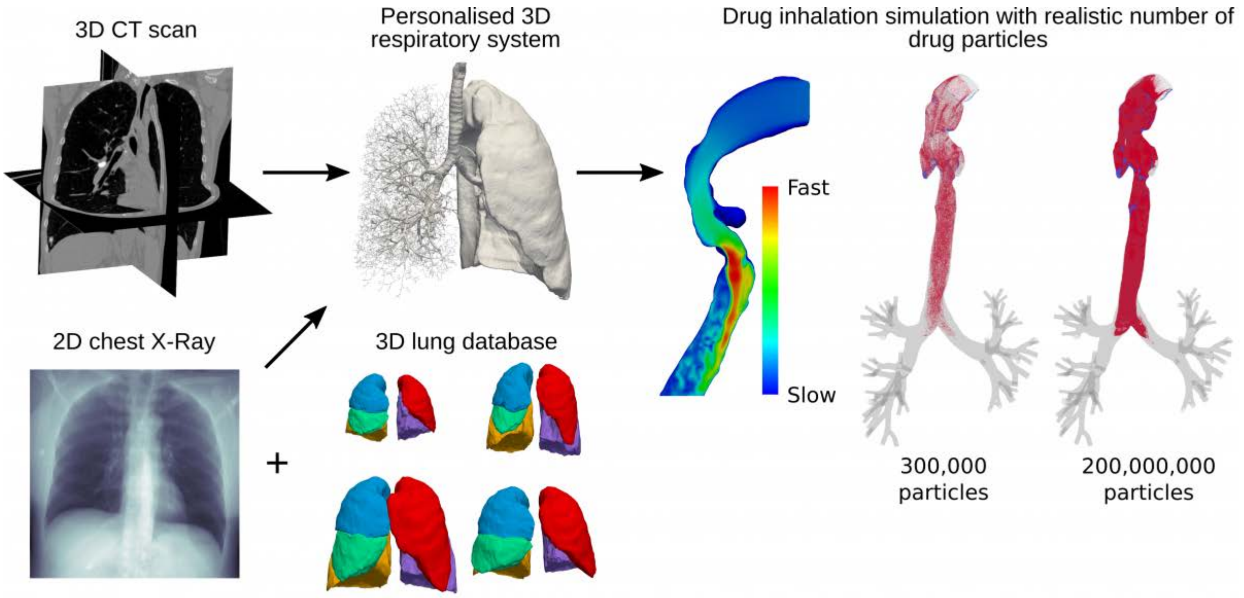
SOLUTION

OCRE funding for advanced aerosol transport modelling

Our project demonstrates cloud computing's benefits provided by OCRE funding for advanced aerosol transport modelling. The cloud access provides us extensive computational resources with implementing various HPC configurations such as across more CPUs than previously with more available RAM that are necessary to perform the first ever simulations of realistic aerosol drug deposition in lung airways. These resources are idle for the code development period but ready for refining models and results that significantly reduce costs for the simulations proposed compared to purchasing and maintaining hardware for our university high performance computing facility. Access to large RAM also supports our medical image processing methods, as our current artificial neural network segmentation tool requires, we significantly down-sample the medical images. Furthermore, as the images only require processed once per patient, having the flexibility of cloud computing allows us to extract high resolution tools without investing in a rarely used piece of hardware.



IMPACT

OCRE funding boosted research on aerosol drugs

The scientific outcomes have been disseminated in scientific journals and conferences on aerosol modelling. The developed computational framework will be released as an open-source software that will be used by other researchers in the field. Data generated here will be used in a later project, which hopefully will be funded by another OCRE funding, to train surrogate models that combine the power of physical models with the speed of neural networks to optimise aerosol drugs. Cloud services will best meet the memory requirements for advancing model training.

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