Boosting CFD simulation of thermal equipment for food processing

by Javier Porto[1], Mónica González[2], Leopoldo Álvarez[3], Ana Palmero[4], Andrés Gómez[5]

1. SDEA Engineering – 2. TACORE – 3. ANFACO-CECOPESCA – 4. INEGI and Faculdade de Engenharia da Universidade do Porto (FEUP) – 5. CESGA

The challenge: developing a specialized tool to simulate thermal sterilization processes in autoclaves

In Europe, the canning industry is important economically, particularly in Spain which is the leading producer of canned fish in Europe, and in Portugal, which is among the top five producers of canned goods. Some of the most energy-consuming processes are the thermal treatments applied in autoclaves for product sterilization, therefore any tool that improves these processes will reduce both energy consumption and CO2 emissions and save costs in the food production chain.

The inherent complexity of the concepts involved in fluid-thermal simulation engineering means that simulation work currently requires the involvement of highly trained and specialized personnel well-versed in these methodologies.

Moreover, the commercial simulation tools currently on the market take a generic approach that makes the representation of the various geometries and operating conditions time-consuming. It is thus a costly endeavour to test products before manufacturing new equipment or putting recipes into production. Therefore, the challenge is to develop a specialized tool to simulate thermal sterilization processes in autoclaves. Fig. 1 shows an autoclave in which multiple processes could be developed. This experiment was developed to address this challenge using technologies such as high-performance computing (HPC) and computational fluid dynamics (CFD) simulation.

From a business perspective for the companies involved in the experiment, this challenge was their first experience with HPC services and, therefore, represented an opening to new competencies and opportunities.

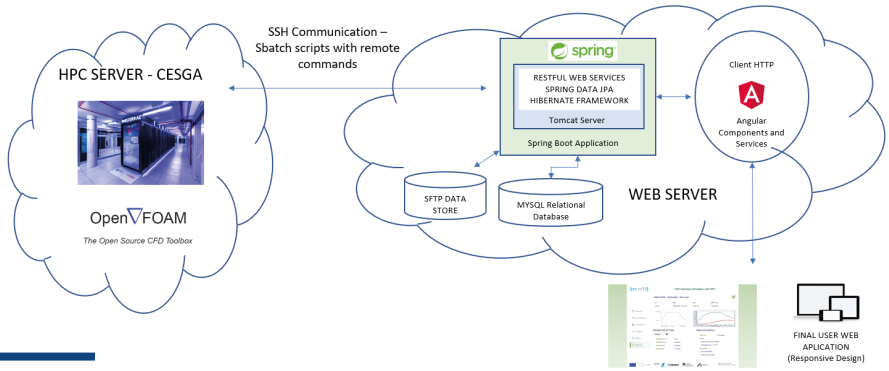

Fig. 1. Multi-process autoclave.

Fig. 2. Web GUI architecture.

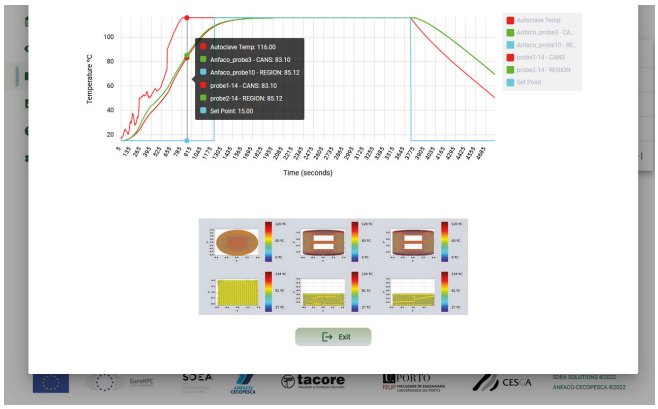

Fig. 3. Simulation example.

The solution: simulation of an autoclave

One solution is a tool specifically for simulating thermal sterilization processes in autoclaves; this tool is a complete SaaS (software-as-a-service) that includes HPC resources and is offered to customers on a subscription basis including all services. It consists mainly of two parts: the simulation model developed using OpenFOAM and executed on the HPC platform, and the Web GUI (graphical user interface) that has the architecture shown in Fig. 2. This application allows users to run simulations of an autoclave, configure certain parameters, and monitor the evolution of the simulation. It also permits the company to analyse previous simulations and compare them with each other.

Without HPC it would take 3–5 hours to run each simulation, which is too long for a good end-user experience. The use of HPC enables autoclave manufacturing companies' end users to run simulations in more detail in less time (between 5–15 minutes per simulation), allowing users to test different cases in a short time.

Fig. 3 shows an example of a simulation output. This Web GUI has the following parts: Login and Registration; Simulation History; Visualization; Simulation and Billing; and Analysis and Configuration. The CFD model, developed with OpenFOAM, has the following features:

- Case study: heat transfer problems between multiple regions
- Mesh: unstructured 3D
- Number of cells: ≈ 1,104,450
- Solver: chtMultiRegionFoam
- Partition method: hierarchical and Scotch

This model is configurable allowing the user to modify more than 30 parameters of the sterilization process, and it was configured to solve the simulation by parallelization to take advantage of the HPC resources, as can be seen in Fig. 4.

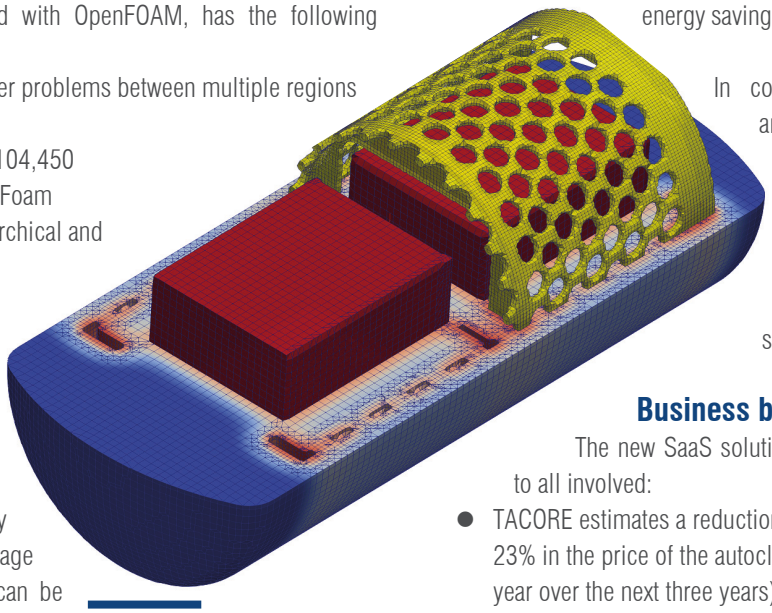

Fig. 4. Simulation mesh.

After validation, some conclusions can be drawn:

- Compared to the use of a computer with comparable medium-level computing resources, execution time was reduced by 90% to processes of 5–6 minutes (300–360 seconds) in length (Fig. 5).
- It seems to establish a knee on the acceleration curve with the following factors: 1 core per task; 48 MPI tasks per node; 8 GB RAM per node.

The results of simulations and validation tests were analysed and the flow rates, pressures, and temperatures of the different fluids in autoclave were studied. This investigation made it possible to compile the energy balance for using the autoclave for sterilizing processes, including the calculation of consumed energy and CO_2 emissions in the final solution, and the effect of including a heat recovery unit in the autoclave.

The SaaS solution: delivering adequate business benefits and significant environmental impact

With the help of the new SaaS solution, partners involved in the experiment could plan their first outputs. TACORE, the end-user in this experiment, gains an advantage in the market from having more efficient and customizable manufacturing. Reducing the costs to develop an autoclave facilitates the replacement of obsolete equipment, leading to an annual saving of €40,000.

For SDEA, the independent software vendor, the new opportunities created will see them incorporating a specialized profile to develop and support the SaaS. The Faculty of Engineering of the University of Porto will introduce this tool to its students as a showcase of the applications with potential for energy optimization. Using this tool, the students can gain knowledge on saving CO_2 emissions.

ANFACO, the technology expert, is using this opportunity to offer a new tool to industries that could apply the new services to their production processes and gain a commercial advantage in terms of energy savings and reduction of CO_2 emissions.

In conclusion, the simulations and analysis of the experiment will provide detailed information on the energy consumption of a machine and identify whether it is possible and useful to take action to reduce it, resulting in a smaller carbon footprint.

Business benefits

The new SaaS solution provides commercial benefits to all involved:

- TACORE estimates a reduction in production costs of around 23% in the price of the autoclave, (less than €100,000 per year over the next three years) representing an annual benefit of 2.7% of the average annual revenue.

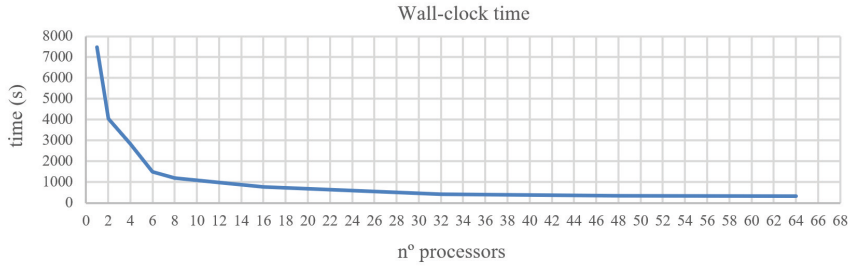

Fig. 5. Clock time vs. number of processors.

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- Cost and energy savings for food companies (ANFACO members and other companies) – an efficiency improvement of 2% would mean a saving of 0.00187592 tCO2/tonne of processed product.
- SDEA estimates an annual income of €40,000–€60,000 for developing a customized application for each new customer opportunity.
- For the Faculty of Engineering of the University of Porto, as an education organization, the main benefit is having a new tool for academic activities and the knowledge gained on HPC and autoclave thermal processes.

This success story was developed during the second tranche of FF4EuroHPC, which supports the competitiveness of European SMEs by funding business-oriented experiments and promoting the adoption of advanced HPC technologies and services.

The experiment is an end-user-relevant case study demonstrating the use of cloud-based HPC and the benefits it brings to the value chain, from the end-user to the HPC-infrastructure provider, thus addressing the business challenges of SMEs by using HPC and complementary technologies such as HPDA (high performance data analytics) and AI. When the experiment is successfully concluded, the result is a success story that inspires the industrial community.

The FF4EuroHPC project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No. 951745. The JU receives support from the European Union's Horizon 2020 research and innovation programme and from Germany, Italy, Slovenia, France, and Spain.

The success story presented in this article was developed during the first tranche of FF4EuroHPC Project. FF4EuroHPC supports the competitiveness of European SMEs by funding business-oriented experiments and promoting the uptake of advanced HPC technologies and services. The experiment is an end-user-relevant case study demonstrating the use of cloud-based HPC (high-performance computing) and its benefits to the value chain (from end-user to HPC-infrastructure provider) for addressing SME business challenges that require the use of HPC and complementary technologies such as HPDA (high performance data analytics) and AI (artificial intelligence). The successful conclusion of the experiment created a success story that can inspire the industrial community.

A Journey through Digital Lung Models

Lung Modelling Congress 2023

The Lung Modelling Congress (www.chiesi.com/lung-modelling-congress/en/) jointly organized by the Centre of Open Innovation & Competence (COI&C) and R&D Digital's Data Modelling Department, took place from November 22–23 at the Chiesi Group Headquarters in Parma in Italy. It gathered together international experts in the simulation of patient airways and respiratory system digital twins from the USA, New Zealand and Europe.

Academics and start-ups shared their best practices, exhibited various excellences, and challenged the current status quo with a roadmap for future developments. The extensive participation and debate confirmed the enormous potential of mathematical models and simulations to shorten time to market, reduce product development costs, personalize real-time diagnoses, and put the patient at the forefront.

This application obviously requires multi-sectoral expertise from various professionals ranging from physicists, mathematicians, and data scientists to pulmonologists and fluid engineers. Open and multidisciplinary events such as the Lung Modelling Congress are therefore key tools for the different communities of researchers and companies to plan future developments in a collaborative and unified manner.

Apart from the design of pharmaceutical products, the development and validation of computational models of the human respiratory system could have a great impact in many areas of healthcare, safety and the environment.

A digital twin of airflow and inhaled drug delivery in a human airway

by Bart De Jong[1], Leonardo Geronzi[2], Marco Evangelos Biancolini[2], Benigno Marco Fanni[3], Simona Celi[3], Gerben Roest[4], Sasa Kenjeres[5]

1. One Simulations – 2. RBF Morph – 3. Fondazione Toscana Gabriele Monasterio – 4. GrepIT – 5. TUDelft

Respiratory diseases such as asthma and chronic obstructive pulmonary disease (COPD) are caused when parts of human airways become narrower. Medical treatment for these diseases involves the patient inhaling drug particles. Some patients experience uneven distribution of the drug particles, resulting in ineffective treatment, increased side effects and wasted medication. At present the deposition of inhaled drugs is studied by having the patient inhale a radiolabelled drug, however, this exposes the patient to a certain level of radiation.

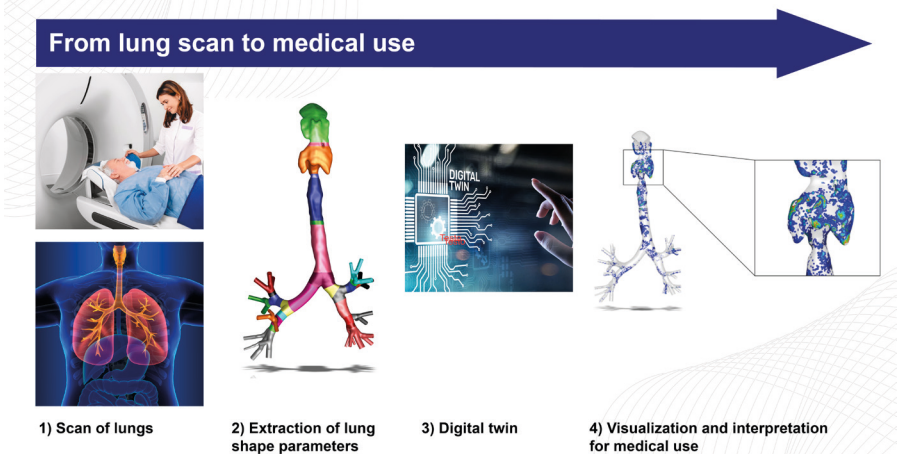

Fig. 1. The concept of the DiTAiD experiment. From left to right: the shape of the patient's lungs is acquired by the scanning device; the image data is processed and the shape parameters extracted; these parameters are used as input to the digital twin of a human airway resulting in a real-time visualization allowing interactive selection of the treatment strategy.

This FF4EuroHPC experiment aims to provide an alternative method whereby a detailed CFD (computational fluid dynamics) simulation is made of the patient. However, conducting a CFD study for each patient would be too complex and time-consuming since it relies on manually creating a 3D model from a CT scan. Even for a CFD expert with access to an HPC (high-performance computing) system, each study would take several weeks to complete, which represents a serious disadvantage for urgent medical cases. The associated costs would also be high.

The solution developed as part of this experiment is an easy-to-use digital twin (DT) that can predict the particle deposition of inhaled drugs in any human airway (Fig. 1). The DT is based on a reduced order model (ROM) that uses mesh morphing technologies on the basic geometry of a human airway to generate 1,000 models of a human airway and then simulates particle deposition using CFD

on a 960-core HPC system. The simulation results are compressed into an ROM, which dramatically reduces the complexity of large-scale numerical simulations while maintaining a good level of detail.

To use the DT, a medical image of the patient's airway is fed into the software, which then automatically extracts its shape parameters and reproduces the results of a CFD analysis from the ROM to assist in optimizing the particle size – all in one click and avoiding time-consuming and expensive CFD workflows.

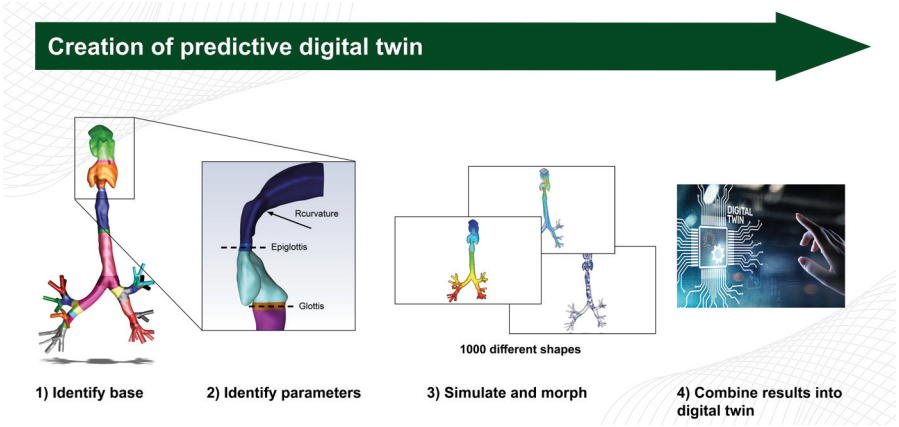

Fig.2. Details of the DiTAiD workflow. From left to right: a basic CFD representing the geometry of an average patient's lung is defined; the geometric parameters of the human airway are identified; mesh morphing is used to study 1,000 different virtual patients; the results obtained are finally combined to create a digital twin that is suitable for representing a specific new patient.

The challenge: creating a predictive digital twin for a human airway

This ambitious endeavour consisted of four major steps (Fig.2), each contributing significantly to the ultimate goal of revolutionizing our understanding of respiratory dynamics and enhancing patient care.

Data preparation and parameter identification

This phase focused on selecting a base geometry of a human airway. To ensure the DT's versatility and applicability to a wide population, the airway was defined using a comprehensive set of shape parameters.

These parameters include vital aspects such as curvature radius, diameter, bifurcation angles, branch lengths, and more. Another equally essential aspect is identifying the flow and particle parameters that are crucial for calculating flow patterns and particle deposition within a human lung. These parameters include inhalation velocity, particle diameter, and particle injection velocity (Fig.1 and Table 1).

Parametric study and data generation

Once the baseline in-silico model representing a generic patient was defined, it had to be prepared for HPC to generate the data required to train the digital twin. A parametric analysis was needed to provide the essential data required to create the ROM and DT.

This phase began with the development of a morphing script, based on RBF Morph technology, to deform the base lung geometry using the shape parameters identified. Simultaneously, a CFD setup was meticulously created in Ansys Fluent for the basic geometry. A rigorous validation study of the CFD setup was conducted in which the CFD results were compared with existing literature. The sensitivity of various parameters, including mesh sensitivity, the number of particle streams to be injected, and other numerical settings were studied.

Once these preparatory steps were completed, a substantial number of CFD simulations – commonly referred to as "snapshots" – were set in motion on an HPC cluster. Each snapshot simulation adapts the basic geometry and mesh to the patient's shape parameters via the morphing script. In addition, the flow and particle input parameters vary for each snapshot within the specified range, following the DoE (design of experiments) table created with the Latin Hypercube Sampling algorithm.

To ensure the quality and reliability of these simulations, an automated script was used for rigorous quality assurance. This meticulous approach eliminated poorly converged runs, paving the way for the subsequent creation of the ROMs.

ROM creation and DT assembly

Once the simulation dataset was generated, the resulting snapshot simulations had to be distilled into invaluable ROMs. Using Ansys Twin Builder, the simulation results were assembled into self-contained ROMs. The

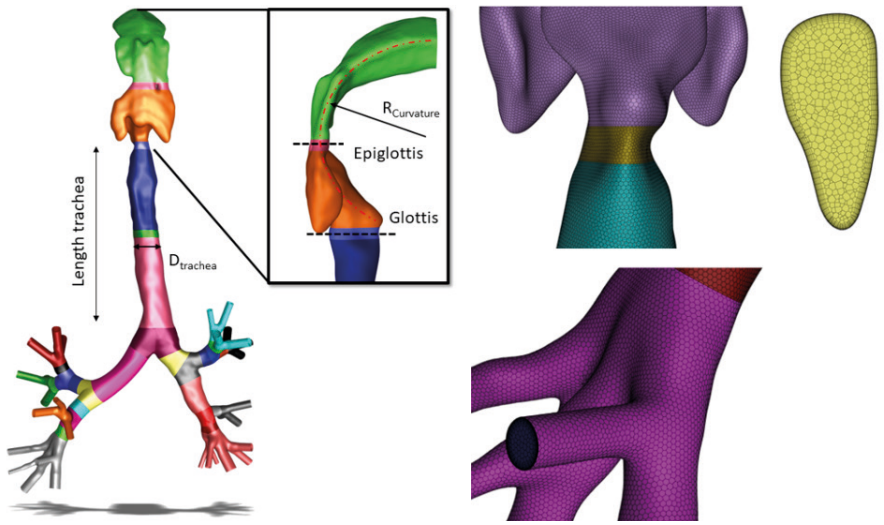

Fig.3. The baseline geometry (left) and its CFD mesh representing a generic patient, ready to receive the parameters of a specific new patient.

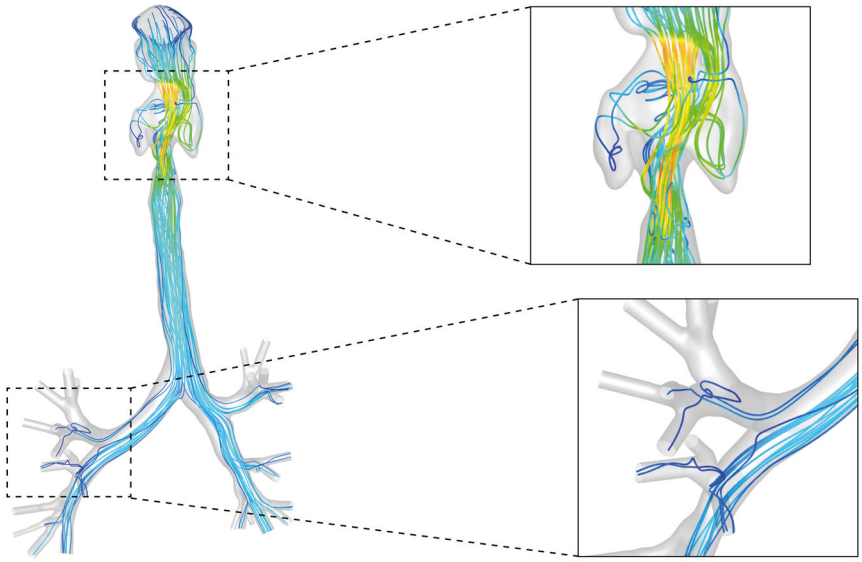

Fig.4. Details of the flow field in a human airway captured by the high fidelity CFD model used in the experiment to represent a generic patient and ready to be adapted to the shape of a specific patient.

accuracy and fidelity of these ROMs were assessed via a rigorous comparison with high-fidelity snapshots. Surprisingly, this comparison revealed minimal differences between the high- and low-fidelity models and those primarily in regions of flow separation, such as near the throat.

The individual ROMs, fast-response models that provide specific flow and particle information, were subsequently amalgamated into a single cohesive digital twin. To facilitate interoperability with other software applications, FMU (functional mock-up unit) files were generated to create an adaptable and robust DT of the human airway.

Revelatory achievements: converting human airways into a predictive digital twin

We began by selecting a fundamental geometry, which was then meticulously prepared for modelling and morphing by CFD. The results are illustrated in Fig.3, which also highlights several key lung shape parameters. The mesh details are also shown.

This process identified a total of 26 lung-shape parameters, each associated with specific ranges of values. The parameters relating to the region of the mouth and throat include the curvature of the throat, the epiglottis, and the glottis. The remaining parameters include the diameter of the trachea, its length, and various lengths and branching angles within the lower portion of the lung.

To streamline the input parameters, we adopted a fixed ratio from the existing literature for the trachea's diameter in relation to the diameters of subsequent branches. Furthermore, we identify three input parameters linked to airflow and drug-particle behaviour: inhalation flow rate, particle diameter, and particle injection velocity. The inhalation flow rate varies between 15L/min and 120L/min, particle diameter fluctuates between 0.1μm and 10μm, and particle injection velocity ranges from 0m/s to 10m/s. An overview of these input parameters and their respective ranges can be found in Table 1.

To achieve optimal spacing between snapshots, a DoE table for 1,000 snapshots was generated using the Latin Hypercube Sampling algorithm.

To create the morphing script, we first extracted the airway centrelines and calculated the shape parameters of the base geometry. Using radial basis functions and the information collected, we transformed the base geometry, thereby generating a new CFD model of a human airway based on each set of shape parameters. In addition, the morphing script generates PTS files that contain the coordinates for each node of the original mesh created using the base geometry along with the node displacements. These PTS files are pre-generated for the entire DoE table and govern the morphing process during the parametric study.

After completing the DoE table, 1,000 CFD jobs were sent to a rented HPC cluster. This cluster consisted of 8 nodes, each with 120 cores, totaling 960 cores for calculations. The purchased Ansys license allowed for 25 simultaneous runs. Unfortunately, 40 runs of the 1,000 submitted jobs failed, and three runs showed poor convergence or unphysical results. These failures were mainly caused by the presence of cells with negative volumes that were generated during the morphing process.

Region of mouth and throat			
$R_{curvature}$ [cm]		2-8	
Epiglottis area [mm^2]		40-400	
Glottis area [mm^2]		40-400	
Region of lower airways			
Generation	**Diameter [mm]**	**Length [mm]**	**Branching angle [deg]**
		Left / **Right**	
0 (Trachea)	15-50	100-120	80-95
1		51-57 / 24-28	75-90
2		12-16 / 15-28	65-95
3		7-10 / 7-10	55-70
Physical parameters			
Flow rate [L/min]		15-120	
Particle diameter [μm]		0.1-10	
Injection velocity [m/s]		0-10	

Table 1: Overview of input parameters and their ranges.

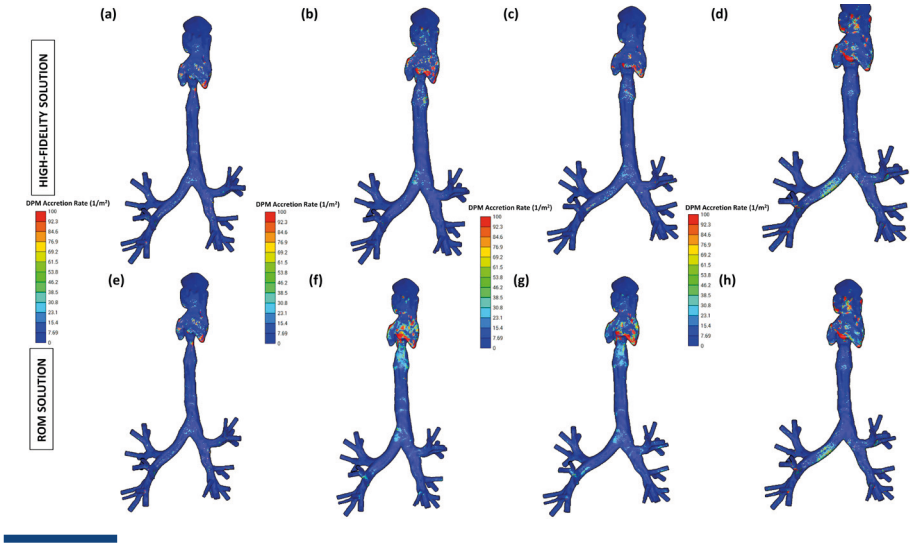

Fig.5. Particle deposition comparison between the high-fidelity CFD simulations (a-d) and the ROM solutions (e-h) for four different virtual patients corresponding to four sets of input parameters.

The snapshot output included data on particle deposition, wall shear stress, velocity, pressure, turbulent dissipation rate (ε), and turbulent kinetic energy (k). For each of these variables, we constructed a ROM. This ROM can calculate results for any combination of the previously defined input parameters, even for combinations that were not simulated in great detail. We quantified accuracy through leave-one-out cross-validation by comparing the low-fidelity ROM results with high-fidelity CFD snapshots not used in ROM creation.

Fig.5 presents a comparison between the CFD and ROM results for drug particle deposition. It reveals the locations in which drug particles are deposited in a human airway in four different scenarios, each characterized by distinct combinations of input parameters resulting in different lung shapes, flow conditions, and particle sizes. The top row shows the results obtained from a CFD simulation, while the bottom row illustrates the results derived from the ROM. The comparison shows minimal differences between the two sets of data. Despite the slight disparities, a ROM can provide results at the push of a button, whereas a full CFD simulation may require weeks. Finally, we consolidated the individual ROMs into a single DT, which was exported in FMU-file format to be accessible by other software applications.

In conclusion, this FF4EuroHPC experiment achieved a ground-breaking milestone in medical science, particularly for the treatment of respiratory diseases such as asthma and COPD. By developing an innovative DT of a human airway, this experiment addressed the critical challenges associated with uneven distribution of inhaled drug particles in patients; exposure to radiation from drug deposition studies; and the time and cost constraints of traditional CFD simulations.
This solution, based on a ROM and mesh morphing technologies, created a versatile and user-friendly tool that can predict particle deposition for any human airway. By automating the process of extracting the shape parameters from medical images, this DT eliminates the need for time-consuming and expensive CFD workflows. This result significantly accelerates the optimization of treatment strategies and improves patient care, particularly for urgent medical cases.

The impact of this research on the medical sector cannot be overestimated. The ability to efficiently and accurately predict drug particle deposition in patient airways not only reduces treatment inefficiencies and side effects, but also minimizes radiation exposure, a significant concern in healthcare. Furthermore, the accessibility of the DT in FMU-file format allows seamless integration with other medical software applications, facilitating collaboration and further research in the field of respiratory medicine.

In essence, this experiment has paved the way for a transformative shift in respiratory medicine by representing human airways in predictive digital twins. This achievement holds great promise for improving the lives of patients suffering from respiratory diseases and underlines the invaluable role of advanced computational modelling in advancing healthcare practices.

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