

Comprehensive Visualization of Large-Scale Simulation Data Linked to Respiratory Flow Computations on HPC Systems

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Abstract

Conditioning large-scale simulation data for comprehensive visualizations to enhance intuitive understanding of complex physical phenomena is a challenging task. This is corroborated by the fact that the massive amount of data produced by such simulations exceeds the human horizon of perception. It is therefore essential to distill the key features of such data to derive at new knowledge on an abstract level. Furthermore, presenting scientific data to a wide public audience, especially if the scientific content is of high societal interest, i.e., as it is the case for fine dust pollution, is not only difficult from a visualization but also from an information transfer point of view. Impressive visual and contextual presentation are hence key to an effective knowledge transfer of complicated scientific data and the involved methods to arrive at such data. In this paper such an approach is presented for highly-dense simulation data stemming from HPC simulations of inspiratory flows in the human respiratory tract. The simulations are performed using a coupled lattice-Boltzmann/Lagrange method and aim at understanding the microscopic interactions of flow and particle dynamics in highly intricate anatomically correct geometries. As such, they deliver insights on the impact of particulate matter on the human body.

1. Scientific story behind the movie

Nowadays, air-dissolved fine dust particles are especially found in urban environments and intensively reduce the air quality. Such particulate matter (*PM*) may originate from various man-made and natural processes and depending on its composition, size, density, and volume fraction They may cause serious physiological and psychological pathologies. Harmful *PM* passing the filtering mechanism of the human nasal cavity and descending into the lung are in general smaller than $10\mu m$. Examples of such particles are Diesel aerosols, nitrogen oxides NO_x , sulphur oxides SO_2 , or unburnt coal particles that stem from, e.g., heavy traffic, coal-fired power plants, or volcanic eruptions. The deposition of such substances acting as free radicals in the human lung can lead to modifications of the genome on cellular level [1]. In case repair mechanisms fail to resolve these issues, cancer can occur. Raaschou et al. [2] found a strong correlation between the frequency of lung cancer associated with air pollution

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Figure 1: Comprehensible visualization of spatial domain decomposition for parallel computation on the BlueGene/Q system JUQUEEN (combined screenshots of section 3 of the movie).

by PMs in the diameter range of $2.5\text{-}10\mu\text{m}$ by correlating air quality measurements and lung cancer statistics in 17 cohorts in 9 European countries. Especially the economical growth in industrial and emerging countries, e.g., in the BRICS-nations Brazil, Russia, India, China, and South Africa, is responsible for the accretion of the world-wide air pollution [3]. A strong increase of fine dust pollution is however also found in developed countries like Germany, e.g., the Stuttgart region suffers from heavy traffic pollution and had to declare states of alert for 22 and 48 days in 2016 and 2017 in the months January to April¹. This trend is also visible in the handbook “Traffic in Numbers”², recently published by the German Federal Ministry of Transport and Digital Infrastructure. It is hence of high societal interest to understand the complex flow in the human respiratory tract and to quantify the deposition behavior of PM to get an estimate of the toxicity of certain substances and how the filtering mechanism of the human body works.

To investigate the influence of PM on a microscopic level, numerical simulations of the flow and the particle dynamics in the human respiratory system are performed at inspiration with a one-sided coupled lattice-Boltzmann/Lagrange method [4]. The simulation software is a hybrid MPI/OpenMP parallelized C++ code and solves the lattice-Bhatnagar-Gross-Krook equation on highly resolved hierarchical Cartesian meshes and the equation of particle motion using Stokes drag. The geometry of the respiratory system down to the first lung bifurcation at the main bronchi stems from a computer tomography (CT) scan of a 56 year old male. The subsequent lung generations up to bifurcation level 12 are generated by the software *Lung4Cer* [5] and glued to the trachea of the CT geometry. The computational mesh is generated by the method described in [6] and contains approximately $2.1 \cdot 10^9$ cells. The computation is performed on 32,768 cores of the IBM BlueGene/Q system JUQUEEN of the Jülich Supercomputing Centre (JSC) and is iteratively advanced for $4 \cdot 10^6$ iterations to cover an inspiration duration of 4 seconds.

The investigations concentrate on the interaction of the highly unsteady flow field and the particle dynamics, especially in transitional regions such as the epiglottis and the larynx region. In this con-

¹Stuttgart alerts <https://www.stuttgart.de/feinstaub>

²Traffic in Numbers http://www.bmvi.de/SharedDocs/DE/Artikel/G/verkehr-in-zahlen_2016.html

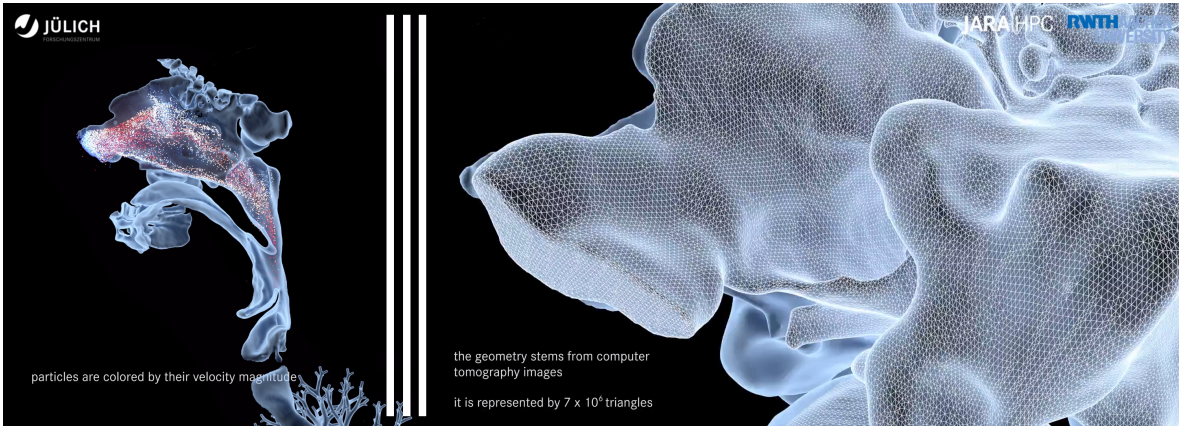


Figure 2: Visualization of simulated particulate matter entering the human respiratory tract (combined screenshots of section 4 of the movie).

text, the impact of associated flow phenomena on the deposition behavior of PM in the upper and lower respiratory tract are of special interest to quantify deposition likelihood of certain PM by lung generation.

2. Enhancement of comprehensibility and interpretability by means of visualization

Extracting scientific insight from large simulations is of crucial importance for science. As mathematician Richard Hamming famously said, "The purpose of computing is insight, not numbers." Especially for nowadays large-scale simulations, which generate a vast amount of data, visualization is one important method to enhance the comprehensibility and interpretability of the results. Scientific evaluation of simulation data is however not the only purpose of rational visualization. Frequently, the preparation of such material for the presentation to the general public is of great importance. This is especially true in societal relevant cases, i.e., in the analysis of the impact of fine dust pollution on human health. Furthermore, research in this area is primarily funded by the public sector demanding for justification *vis à vis* the taxpayer. Therefore, it is indispensable to present a topic that effects everyone in a meaningful way and to hide the complexity of the applied methods and models behind a comprehensible transcript such as a movie.

In this sense, the movie is rather for the general public than for scientific evaluation. It can be grouped into four sections. In the first 24 seconds the viewer shall be convinced that the presented topic is of personal importance. This ensures a high degree of attention and interest in the movie. The next 38 seconds are about introducing the viewer to the complex geometry of the human respiratory tract. Here the movie presents background information and is on purpose not overloaded with information to make sure that the viewer is able to take in what is being shown. In the following 24 seconds the necessity of HPC is discussed with great visual impact (fig. 1). The intention of this section is to convince the viewer that HPC matters. In the last seconds a short view on the simulation results is given (fig. 2). It shows how PM enters the nose and travels through the complex geometry of a respiratory tract. Overall, this movie shall support the statement "HPC Matters" in a sense that viewers can extend it to "HPC Matters for my personal life".

3. State-of-practice

The first step to create the movie starts with extracting meaningful data from the large-scale data sets generated for each time step. Here serial I/O or data filtering are not feasible to process the vast amount of data. Therefore, the simulation software makes use of the *parallel netCDF* [7] library to write the adapted mesh refined (AMR) data to disk.

For an initial parallel visualization of the AMR data in *ParaView*³, the computational mesh and a solution file are subsequently read. A specific parallel ParaView reader is linked against the partitioning algorithm of the simulation software [6]. Internally, a `vtkUnstructuredMesh` and the according halo cells are generated. To visualize the data multiple ParaView servers run on the visualization nodes of the supercomputer JURECA at JSC, each containing two NVIDIA K40 GPUs. Any need to move the data files can be avoided as the computational resources for visualization are fully integrated into the supercomputer. Remote desktop sessions are easily accessible via TurboVNC and, with server-side rendering over VirtualGL, through the user interface *Strudel*⁴.

The movie is compiled and rendered with *Blender*⁵. Therefore the geometry data is converted to STL and read with Blender while the simulation results are preprocessed in ParaView and converted to X3D before they are integrated into the scene. The final rendering is scripted and computed as batch job in parallel with multiple Blender instances on JURECA.

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³ParaView <http://www.paraview.org>

⁴Strudel <https://www.massive.org.au/>

⁵Blender <http://www.blender.org>