81. Latvijas Universitātes starptautiskā zinātniskā konference 2023

UNIVERSITY OF LATVIA

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FACULTY OF PHYSICS, MATHEMATICS AND OPTOMETRY

81st International Scientific Conference

University of Latvia

VIRTUAL MODELS FOR SUSTAINABLE AND SAFE LIVING ENVIRONMENT

Book of Abstracts

Latvijas Universitātes

81. starptautiskā zinātniskā konference

Virtuālie modeļi ilgtspējīgai un drošai dzīves videi

Tēžu krājums

2023

University of Latvia. 81st International Scientific Conference, Virtual Models for Sustainable and Safe Living Environment: Book of Abstracts. Riga: University of Latvia, 2023. 14 lpp.

The 81st International Scientific Conference of the University of Latvia.

Virtual Models for Sustainable and Safe Living Environment.

Book of Abstracts

Latvijas Universitātes 81. starptautiskā zinātniskā konference.

Virtuālo modeļu ilgtspējīgai un drošai dzīves videi sekcija.

Tēžu krājums

Tēžu krājums publicēts autoru redakcijā

Sastādītāja: Daiga Cepīte-Frišfelde

DOI: https://doi.org/10.22364/luszk.81.vimo.ab.

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Virtual Models for Sustainable and Safe Living Environment

Friday, 27th January **2023, 1.00 PM**, Riga

Programma/Programme

Vadītājs/Chair: Vadims Geža		
13.00–13.15	**Jurijs Ješkins** *University of Latvia*	**Augstās veiktspējas skaitļošana kā pētniecības rīks – iespējas un izaicinājumi** High performance computing as a research tool – opportunities and challenges
13.15–13.30	**Kirils Surovovs, Jānis Virbulis** *University of Latvia*	**Hidrodinamisko aprēķinu ar OpenFOAM efektivitātes testēšana uz HPC klasteriem** Testing of the efficiency of OpenFOAM hydrodynamical simulations on HPC clusters
13.30-13.45	**Kristers Kokars[1], Armands Krauze[1], Jānis Oliņš[2], Aleksandrs Gutcaits[3]** [1] *University of Latvia* [2] Ltd. *Castprint* [3] *Riga Technical University*	**Lūzumu ārstēšanas 3D drukāto fiksatoru topoloģiskā optimizācija ar galīgo elementu programmatūru** Topological optimization of 3D-printed fracture treatment casts with finite-element software
13.45-14.00	**Andris Avotiņš** *University of Latvia* *Institute of Food Safety, Animal Health and Environment "BIOR"* *Latvian Ornithological Society*	**Piemēri biodaudzveidības un augšņu izplatības modelēšanā LU SMI klāsterī** Examples of biodiversity and soil distribution modelling with LU SMI cluster
14.00-14.30	**Kafijas pauze, diskusijas** **Coffee break, discussions**	

14.30–14.45	**Uldis Bethers, Juris Seņņikovs, Andrejs Timuhins** *University of Latvia*	**Klimata indikatoru nākotnes projekcijas Lietuvai** Climate indicator future projections in Lithuania
14.45–15.00	**Aigars Valainis, Vilnis Frišfelds, Daiga Cepīte-Frišfelde** *University of Latvia*	**Viļņu klimata reanalīze Rīgas jūras līcī** Reanalysis of wave climate in gulf of Riga
15.00-15:15	**Jānis Bikše[1], Inga Retiķe[1], Ezra Haaf[2], Andis Kalvāns[1]** [1] *University of Latvia* [2] *Chalmers University of Technology*	**Pazemes ūdens līmeņu laikrindu aizpildīšana iekļaujot iztrūkstošo vērtību raksturu** Groundwater level time series imputation considering missing value patterns
15.15-15.30	**Maksims Pogumirskis, Tija Sīle** *University of Latvia*	**Zemā līmeņa strūklu automātiska identificēšana atmosfērā Kurzemes piekrastē** Automatic identification of low-level jets in atmosphere near coast of Kurzeme
15.30-15.45	**Dagis Daniels Vidulejs, Andrejs Sabanskis** *University of Latvia*	**Gaisa attīrīšanas iekārtas efektivitātes novērtēšana dažādos apstākļos** Evaluation of the efficiency of an air purification device in different conditions
15.45-16.10	**Kafijas pauze, diskusijas** **Coffee break, discussions**	
16.10-16.30	**Noslēgums, diskusijas** **Conclusions, discussions**	

SATURS

HIGH PERFORMANCE COMPUTING AS A RESEARCH TOOL – OPPORTUNITIES AND CHALLENGES

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High Performance Computing (HPC) refers to the use of powerful computer systems to perform complex calculations and simulations in a short amount of time. This technology is crucial for modern science, as it enables researchers to analyze and model large sets of data and make predictions about natural phenomena.

One of the main applications of HPC in modern science is in the field of weather forecasting. Using HPC, scientists can simulate the atmosphere and predict weather patterns with a high degree of accuracy. This is important for a wide range of industries, including agriculture, transportation, and energy production. For instance, a study by Zhang et al. (2017) used HPC to simulate the dynamics of a severe thunderstorm, providing new insights into the physics of these weather systems.

Another important application of HPC is in the field of molecular dynamics. This technique is used to study the behavior of molecules and chemical reactions at a microscopic level. By simulating these processes on a computer, scientists can gain a better understanding of how molecules interact and develop new materials with specific properties. A recent study by Li et al. (2019) used HPC to simulate the mechanical properties of a new class of superhard materials, providing valuable information for the development of new cutting tools.

HPC is also used in the field of biotechnology and bioinformatics. For example, scientists can use HPC to analyze large amounts of genetic data to identify patterns and identify potential targets for drug development. A study by Chen et al. (2018) used HPC to analyze the genetic data of thousands of cancer patients, providing new insights into the underlying mechanisms of the disease.

Despite the many benefits of HPC, there are also some challenges that must be addressed in order to fully realize its potential. One of the main challenges is the cost of HPC systems, which can be quite high. Additionally, the high power consumption of HPC systems can be a concern in terms of energy efficiency and environmental impact. As reported by Li et al. (2020) in their study, the energy consumption of HPC systems is a critical issue that needs to be addressed in order to sustain the development of HPC.

Another challenge is the complexity of HPC systems. These systems often require specialized software and expertise to operate and maintain, which can be a barrier for many researchers. A study by Usman et al. (2023) highlighted the importance of HPC systems in big data analysis. The explosion of data from multidisciplinary domains will demand powerful HPC systems with efficient resource management.

In conclusion, High Performance Computing is a powerful tool that can help scientists make new discoveries and solve complex problems in a variety of fields. However, challenges such as cost, power consumption, and complexity must be addressed in order to fully realize the potential of HPC in modern science.

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Li, J., Liu, Z., & Wang, Y. (2019). High-performance computing simulations of superhard materials. Journal of Materials Science, 54(4), 3278-3288.

Chen, Y., Wang, X., & Li, J. (2018). High-performance computing in bioinformatics and biotechnology. Journal of Biotechnology, 260, 17-26.
Li, J., Liu, Z., & Wang, Y. (2020). High-performance computing and energy efficiency. Journal of Computational Science, 34, 101104.
Usman, S., Mehmood, R., Katlib, L., Albeshri, A. (2023). Data locality in high performance computing, big data, and converged systems: an analysis of the cutting edge and a future system architecture. Elecxtronics, 12(1), 53.

TESTING OF THE EFFICIENCY OF OPENFOAM HYDRODYNAMICAL SIMULATIONS ON HPC CLUSTERS

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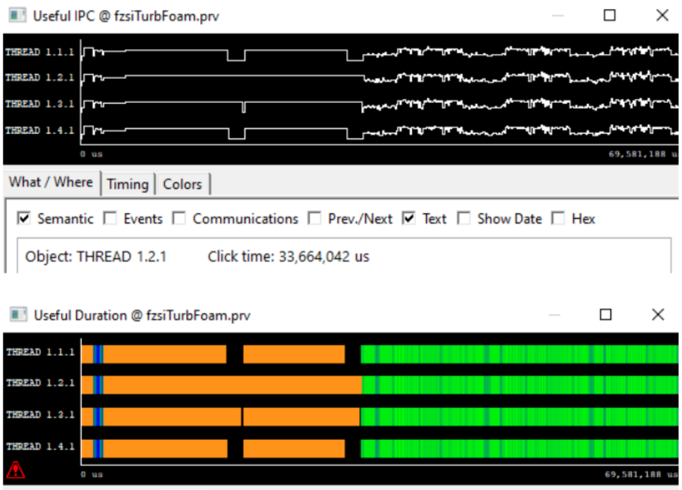
Nowadays, high-performance computing (HPC) is gaining popularity both in industrial and scientific applications. Due to the large number of problems to be solved, computational resources are still limited despite developments in hardware design. Therefore, it is important to ensure that the limited resources are used efficiently.

There are several ways to describe the efficiency of HPC simulations. One of them is using the metrics proposed by the Performance Optimisation and Productivity (POP) center [1]. These metrics include not only global efficiency (which can be evaluated simply by running a simulation and measuring its execution time), but also allow to analyze its components. Some examples are parallel efficiency (how well the computational load is balanced between threads, how much time is spent on the communication between them) and computation scalability (how much the number of instructions increases when more cores are used). To obtain the POP metrics, the following open-source tools are available: *extrae* for trace creation, *paraver* and *basicanalysis* for trace analysis and results' visualization [1].

The present work describes the efficiency tests of hydrodynamical simulations performed on LU [2] and RTU [3] clusters using an open-source C++ library OpenFOAM. The results of different OpenFOAM versions are compared. In addition, different mesh sizes were tested and the influence of simulation decomposition on multiple nodes was analyzed. A previously known rule-of-thumb of using 10 000 mesh elements for one thread has been affirmed.



	843 000 (standard)			
Number of processes	2	4	8	16
Global efficiency	96.9	106.4	91.1	74.3
Parallel efficiency	96.9	92.0	84.2	72.7
Load balance	98.8	98.8	93.7	89.9
Communication efficiency	98.1	93.1	89.9	80.9
Serialization efficiency	100.0	100.0	100.0	100.0
Transfer efficiency	98.1	93.2	89.9	81.0
Computation scalability	100.0	115.6	108.2	102.1
IPC scalability	100.0	116.8	115.8	108.2
Instruction scalability	100.0	98.4	98.1	100.6
Frequency scalability	100.0	100.6	95.2	93.9
Speedup	1.0	2.2	3.8	6.1
Average IPC	1.7	2.0	1.9	1.8
Average frequency (GHz)	3.9	3.9	3.7	3.7

Fig. 1. Examples of the obtained results: different views of *extrae* trace visualized by *paraver* (left) and a table of POP efficiency metrics obtained by *basicanalysis* (right).

References:

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[2] https://modinst.lu.lv/en/pakalpojums/augstas-veiktspejas-aprekini/
[3] https://hpc.rtu.lv/?lang=en

TOPOLOGICAL OPTIMIZATION OF 3D-PRINTED FRACTURE TREATMENT CASTS WITH FINITE-ELEMENT SOFTWARE

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Modern methods of treating bone fractures involve 3D printed plastic casts, which have multiple advantages over traditional plaster fixators. Holes are formed in the casts to increase ventilation, lower material cost and printing time, while preserving as much mechanical and structural integrity as possible. Optimization of the cast topology is needed to obtain optimal hole shapes and placement in the cast.

In this work, a numerical implementation of a fixator topology optimization algorithm is presented. The algorithm is implemented as a script written in FreeFEM [1]. The goal is to design an automatic procedure that includes the topologic optimization of the casts on an HPC cluster in the production chain of the 3D printed casts which would improve the quality and reduce the overall production time and price.

Density-based topology optimization is used in the script. It optimizes the total deformation energy under mechanical stresses caused by either surface or volume forces, which model contacts at one or several points and material bending, respectively. Additionally, a penalty method ensures that the total filled volume reaches a specified value.

A series of simulations were performed on the RTU HPC Center infrastructure. Various force application schemes were tested, which resulted in vastly different material topologies. The force configuration needs to provide a solution that is both viable and is based on stresses that appear in actual use. Some promising optimized geometries were obtained and have already been printed by SIA CastPrint for validation.

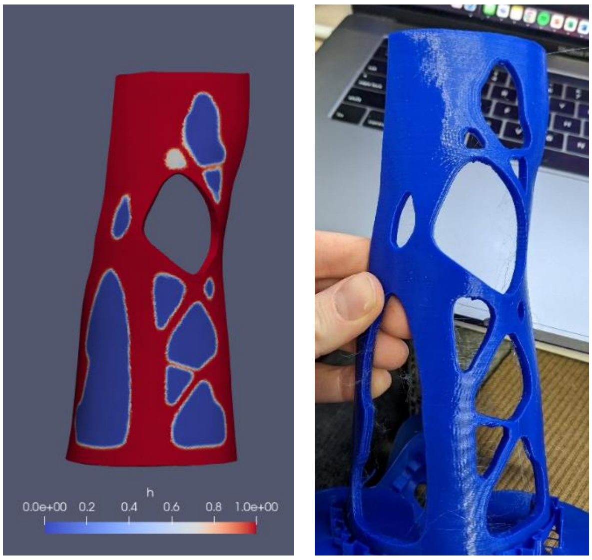

Fig. 1. Optimization result and the respective print.

References:

[1] Hecht, F., 2012. New development in FreeFem++. Journal of numerical mathematics, 20(3-4), 251-266.

EXAMPLES OF BIODIVERSITY AND SOIL DISTRIBUTION MODELLING WITH LU SMI CLUSTER

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Data analysts in the fields of geography and biogeography often face datasets larger than available rapid access memory (RAM) or computational processes lasting for a long time (days or even months) if processed on a single core. In this presentation, I provide examples of approaches used in biodiversity and soil distribution modelling with the University of Latvia Institute of Numerical Modelling (LU SMI) cluster and the designated virtual machine within it.

The first example illustrates the speed gain and efficient use of RAM when utilising Apache Arrow © for structured data useful both on cluster and desktop machines. The second example introduces approaches used in the evaluation of river and dam importance for fish species, combining parallel processing and an example of a situation when spatial subsetting is not possible (HydroDEM). Finally, I will present the workflow of peat soil distribution analysis combining LU SMI cluster (for data from national databases processing and model selection) with Google Earth Engine (for model prediction and remote sensing data processing).

In conclusion, cloud computing is an important asset when dealing with geographical data analysis.

REANALYSIS OF WAVE CLIMATE IN GULF OF RIGA

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We performed wave climate calculation in the Gulf of Riga by using 3-rd generation wave model SWAN [1]. The calculation covers period from 1993 till 2020 and provides a dataset with hourly data for significant wave height, wave period and wave direction and energy flux. Model is implemented on regular spatial grid with 2km step. Directional resolution in wave spectrum is 6 degrees and it covers wave frequency spectral range of 0.05-0.5 Hz with 24 grid points.

As wave calculations on climatic scale for the Baltic Sea have been done before [2], our approach includes considering local ice conditions.

Model forcing is provided by ERA5 [3] the fifth generation ECMWF reanalysis for the global climate and weather. Wave boundary condition are obtained from Baltic Sea Wave Hindcast [4] based on the wave model WAM cycle 4.6.2., or alternatively by using of Fetch algorithm. These boundary conditions are applied on W and N borders of Gulf, Irbe and Suur strait respectively.

While ice conditions are calculated by climatic model based on operational oceanographic model of University of Latvia (in turn based on HIROMB-BOOS).

Our calculation allows estimations on wave energy in coastal zones and ice condition influence on said energy flux. Special attention had been paid to eastern coast of the Gulf of Riga up to 20 m depth.

Acknowledgements:

The work has been carried out within the framework of the CE2COAST project funded by Ministry of Education and Science, Republic of Latvia through the 2019 “Joint Transnational Call on Next Generation Climate Science in Europe for Oceans” initiated by JPI Climate and JPI Oceans. Contract No. 23-11.17e/20/246.
The wave energy in coastal zone of the eastern shore of the Gulf of Riga has been assessed implementing the depth profiles acquired by Latvian Institute of Aquatic Ecology during its monitoring works in summer 2022.

References:

[1] https://swanmodel.sourceforge.io/download/zip/swantech.pdf
[2] Soomere, T., 2021, Numerical simulations of wave climate in the Baltic Sea: a review, Oceanologia
[3] https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-single-levels?tab=overview
[4] https://data.marine.copernicus.eu/product/BALTICSEA_REANALYSIS_WAV_003_015/

GROUNDWATER LEVEL TIME SERIES IMPUTATION CONSIDERING MISSING VALUE PATTERNS

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Groundwater hydrographs, similar to any time series, have missing values as a result of uneven measurement frequencies, technical malfunctions, or human-made errors. A variety of automated gap imputation methods are applied when dealing with regional-scale data sets, but the assessment of simulation performance remains a challenge and is commonly performed by randomly introduced missing values. Yet, groundwater level time series rarely have random gaps and more complex gap patterns can be observed. Do the missing value patterns of a data set affect the imputation performance? And how could we improve the assessment of imputation methods? These were among the main questions of this study.

We present a new artificial gap introduction technique (TGP - typical gap patterns) mimicking realistic gap patterns characteristic for regional-scale groundwater hydrographs. The approach applies to any type of time series to improve the imputation assessment based on the complexity of gaps in a particular data set. Machine learning algorithms missForest and imputePCA were compared with routinely used linear interpolation to infill up to 2.5 years-long gaps in groundwater level time series covering all three Baltic states. While the missForest algorithm significantly outperformed imputePCA and linear interpolation, they often tend to fail to impute previously unseen extremes (such as drought events in 2018) and anthropogenically affected time series (potentially due to water abstraction near cities).

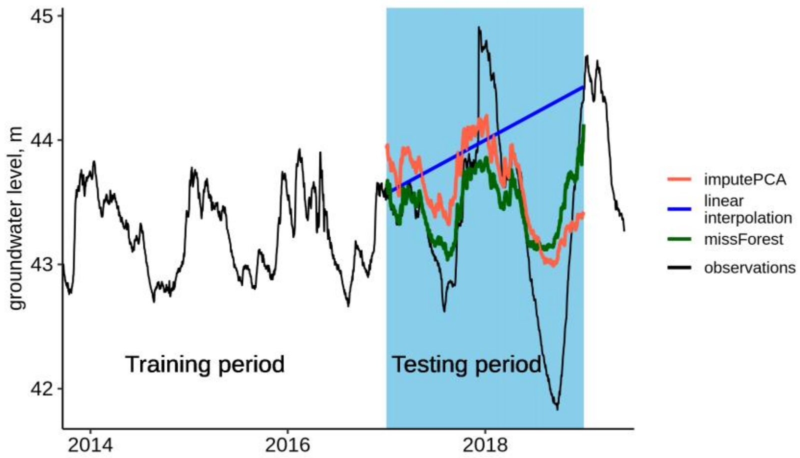

Fig. 1. Example of modelled artificial gap in groundwater level hydrograph (blue shaded area) for Estonian well No. 1156 where extreme drought event has not been properly imputed.

Acknowledgements:

This research is funded by the Latvian Council of Science, project “Spatial and temporal prediction of groundwater drought with mixed models for multilayer sedimentary basin under climate change”, project No. lzp-2019/1-0165; Ministry of Education and Science, Latvia and University of Latvia grant No. ZD2016/AZ03 “Climate change and sustainable utilization of natural resources”. The research further contributes to grant TRV2019/45670 awarded by the Swedish Transport Administration(Trafikverket).

AUTOMATIC IDENTIFICATION OF LOW-LEVEL JETS IN ATMOSPHERE NEAR COAST OF KURZEME

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A low-level jet is a maximum in the vertical wind speed profile in the lowest layers of atmosphere. Low-level jets, when present, can have a significant role in the wind energy. An increased wind speed in the rotor plane of the wind turbines can increase their electrical energy production. However, low-level jets can put uneven load on the blades of the turbine, which can lead to their damage. Several recent studies have shown the presence of low-level jets near the coast of Kurzeme. Typically, the wind speed maxima of the low-level jets are located at the height of several hundred metres. Meanwhile, the wind speed maximum of low-level jets near the coast of Kurzeme is within the lowest 100 metres of the atmosphere.

In this work data from UERRA reanalysis on 12 height levels in the lowest 500 metres of the atmosphere is used to automatically identify low-level jets. A region between coast of Kurzeme and Gotland is chosen as the area of interest. At first, an algorithm that is widely used in literature to estimate frequency of low-level jets was applied. The algorithm seeks for maximum in the vertical wind speed profile in the lowest 150 metres followed by an inversion of temperature above the jet maximum. The frequency of low-level jets was calculated, grouping events by the wind direction, which allowed to identify main trajectories of the low-level jets. For further analysis, several vertical cross-sections of the atmosphere, that low-level jets frequently flow through, were chosen. Meteorological parameters were interpolated from model grid to the cross-section grid.

To investigate mechanisms behind low-level jets, Principal Component Analysis (PCA) was applied to the cross-section data of wind speed, temperature and geostrophic wind speed to identify main patterns of these meteorological variables. Diurnal and seasonal cycles of these patterns as well as correlations between patterns of different meteorological parameters were analysed to gain better understanding of mechanisms behind low-level jets in the region.

EVALUATION OF THE EFFICIENCY OF AN AIR PURIFICATION DEVICE IN DIFFERENT CONDITIONS

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Since 2021, air purifiers have been recommended for reducing airborne infectious aerosol exposure by organizations such as WHO and ASHRAE [1,2]. However, for an efficient indoor air purification, it is important to consider the airflow in the room. In this work we investigate the influence of the heating conditions, device orientation and air pollutant source location on the purification efficiency. A large number of fluid dynamics and aerosol transport simulations are conducted using the software OpenFOAM, a few different cases are shown in Fig. 1. The results of this study are used to improve the prototype device design, which is currently under development.

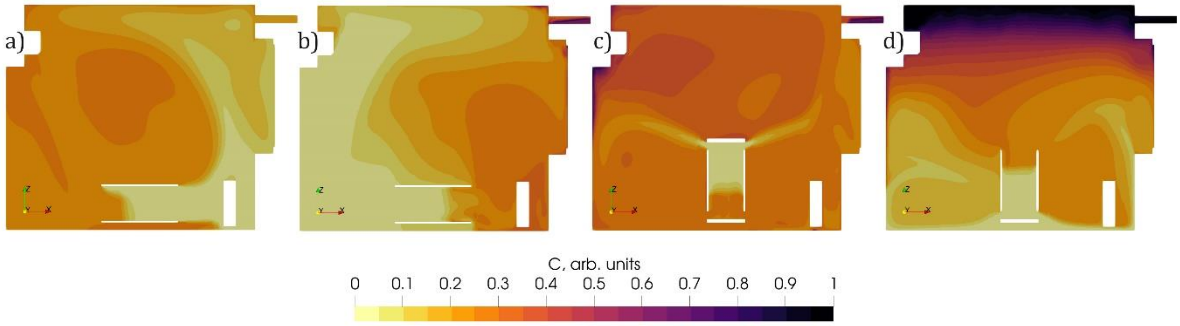

Fig. 1. Concentration distributions in the 3x3x3 m^3 room after 400 seconds, starting with a uniform $C_0 = 1$. Four different air cleaner cases with four different heating regimes are shown. Case a) the room is heated by an air-air heat pump / conditioner and purifier flow is in +x direction; case b) heated floor and purifier flow in -x direction; case c) radiator and upward purifier flow with top lid; case d) heated ceiling and downward purifier flow direction.

A popular metric for rating an air cleaner's efficiency is the clean air delivery rate (CADR) measured in m^3/h, recognized by WHO and EPA. The CADR can be used to quantify an air purifier's performance in a typical house room - the standard measurement chamber is 28.5 m^3 and the simulated room is 27.3 m^3. It was found that the actual CADR value of the purifier can vary drastically in different conditions. The average CADR value was only 373.3 m^3/h, compared to the rated CADR of 723.6 m^3/h based on airflow and filtration efficiency. Horizontally oriented purifier variants were found to be less consistent and poorer in performance than the vertical variants.

Acknowledgements:

The present research has been supported by the European Regional Development Fund, Project No. 1.1.1.1/21/A/046.

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