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MicroLabVR: A VR-Based Platform for Interactive 3D Microbiome Data Visualization

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Abstract. Microbiome data are inherently complex, high-dimensional, and often challenging to interpret using conventional two-dimensional visualization techniques. To address this limitation, we present MicroLabVR, a proof-of-concept virtual reality (VR) application designed for the immersive visualization and exploration of simulated microbiome data. MicroLabVR supports the interactive inspection of spatial population dynamics and substance concentration distributions in two and three dimensions, offering a more intuitive understanding of microbial behavior. The application integrates data exported from BacArena, a hybrid constraint- and agent-based modeling tool, and visualizes metabolic fluxes and explores spatiotemporal changes within a simulated Petri dish environment. Unlike existing microbiome visualization tools, MicroLabVR enables real-time exploration of dynamic, spatially resolved simulation data in an immersive 3D environment. It provides a novel interface that enhances the interpretation of microbiome simulations by allowing users to interactively examine spatial patterns, temporal changes, and metabolic activities. Future developments will focus on volumetric representations, integration of metabolic flux directions, and streamlined data transfer from simulation tools. MicroLabVR extends the capabilities of existing desktop platforms and highlights VR's potential in microbiome research.

1 Introduction

Microbiomes play a vital role in natural environments and for humans, providing diverse ecosystem services from biodegrading waste and digesting nutritious food to protecting higher organisms from pathogens through immune barriers [1, 2]. The development of omics methods such as metagenomics [3, 4], metatranscriptomics [5, 6], and others [7–10] have paved the way to a precise assessment of microbiomes' composition and activity. Drawing on such data, researchers have developed mathematical models detailing microbial growth dynamics to help elucidate processes driving their dynamics. [11–13]. Constraint-based modeling (CBM) and agent-based modeling (ABM) are widespread approaches. CBM is

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based on flux balance analysis (FBA), which can model metabolic processes and the growth of individual microbial species. By coupling multiple species models to a shared environment, crossfeeding interactions between organisms within a community can be simulated. To be able to capture dynamic changes in microbiomes, dynamic FBA (dFBA) has been developed [14]. In such a dFBA model, time proceeds stepwise, and in each step, environmental substance concentrations are first used to predict the growth of individual species. Predicted microbial growth rates are then used to update biomass concentrations, and predicted uptake and secretion fluxes of each species model are used to update environmental substance concentrations. Mathematically, FBA is an optimization problem that calculates the optimal metabolic flux distribution that enables maximal growth for an individual microbial species [15–17].

The dFBA approach can be extended to a spatial domain as well. It discretizes space into small, well-mixed compartments such that the dFBA approach can be applied to each compartment individually. Spatial processes such as diffusion of substances and the migration of microbial cells are then considered separately in the simulation loop [18]. Developing spatial gradients can then influence the migration of organisms, allowing for the investigation of spatial behavior [13, 19].

Contrary to the use of FBA, which analyzes mean metabolic behavior averaged over many cells, ABM focuses on the individuals of a microbial community, capturing population heterogeneity by considering each microbial cell as an individual "agent". ABM models do not rely solely on stoichiometric data but assign properties and behavioral rules to these agents that influence the global development of a microbiome [13, 20–22]. Rules that reflect individual properties or environmental conditions can also guide the simulation. [23, 24].

Spatiotemporal simulation models following the ABM paradigm produce large amounts of data which are challenging to visualize properly. Datasets with multiple dimensions are difficult to interpret on a computer monitor [25]. Additionally, many modeling tools lack a graphical user interface [13, 26], making them accessible only to experts with programming expertise. This requirement poses a barrier for numerous scientists who may not have sufficient coding experience [27–29]. Virtual reality (VR) can overcome this weakness by creating a more flexible, immersive, and interactive environment [25, 30, 31].

This paper investigates which visualization methods are most suitable for presenting simulated spatiotemporal microbiome datasets in VR, what benefits users can derive from a VR application compared to a desktop application, what challenges may arise during the development of such an application, and possible solutions.

This paper presents a proof-of-concept VR application named "MicroLabVR", which visualizes datasets generated by microbiome simulation tools such as BacArena [13]. MicroLabVR is the first tool of its kind to combine spatially explicit, temporally resolved microbiome simulation data with interactive, immersive 3D visualization in VR. It uniquely supports the inspection of metabolic fluxes, microbial movement, and concentration gradients in a unified, manipulable environment, thereby facilitating a more intuitive analysis of complex simulation outcomes. Section 2 outlines how BacArena [13] works and common methods for visualizing microbiome datasets. Section 3 describes the dataset generation process, the required structure for MicroLabVR compatibility, and how we tested the VR application's performance. The next two sections cover the implementation and performance test results, followed by a discussion in Section 6 and a conclusion with an outlook on future improvements in Section 7.

2 BacArena and Visualization Techniques

Studies on modeling software have shown its potential, resulting in a variety of tools available for researchers. We examine BacArena [13] by presenting its features and successful applications in research so far.
BacArena [13] is a hybrid modeling tool, combining CBM and ABM, available as an R extension package. It allows the simulation of mixed communities in a two-dimensional (2D) simulation domain. Population dynamics can change the distribution of organisms throughout the simulation. Influenced by substance concentrations, organisms move towards food sources and replicate into neighboring grid cells. These concentrations decrease because of consumption or increase because of production by surrounding organisms. The rate at which environmental concentrations change depends on the metabolic network of the involved organisms, as determined by FBA predictions. All time steps can be visualized as separate 2D plots showing either the population (see Figures 1) or the substance development. Both figures are based on a simulation using the simplified human intestinal microbiota (*SIHUMI*), consisting of seven microbial species.

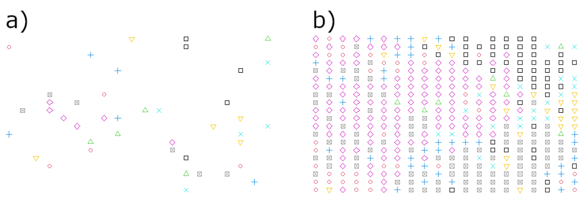

Figure 1. Image a) shows the population after two hours, and image b) after eight hours (created with BacArena [13])

Bauer et al. [13] modeled the arrangement of a variety of phenotypes in a Pseudomonas aeruginosa biofilm. The formation occurred via identified cross-feeding interactions, which resulted from the presence of fermentation end products of fermentation processes. In the same study, they investigated seven species of bacteria in a *SIHUMI* model. Their behavior was characterized by an imbalance in mucus glycan availability, resulting in a localized growth of bacteria that could degrade them. They deduced that such metabolic gradients shape microbiota compositions, leading to proposals about the active restoration of human gut health. One hypothesis stated by Bauer et al. was that a change in eating behavior or metabolic interventions may have a more positive effect than immunosuppressants [13].
When analyzing data, clear and intuitive visualization is important for the user's perception [32]. Heatmaps, as used in BacArena [13], can improve the interpretation of intensity values but are limited by their 2D nature, especially if users explore temporal changes. Moore et al. [33] made approaches to using spatial perception, as they developed a tool that provides a 3D heatmap visualization of multidimensional microbiome data.
However, conventional desktop screens can still only depict spatial data on a 2D surface, limiting depth perception. VR simulations add the effect of immersion to a 3D environment, resulting in a better understanding of data spaces and spatial references [30–32]. Spatial relationships are significant when it comes to metabolic networks. A VR interface, combined with a desktop view by Aichem et al. [34], benefits from the strengths of both approaches. While VR offers a 3D visualization and spatial manipulation of the data points to view the network from different perspectives, the desktop interface is a backup for people who are prone to cybersickness [34].

3 Methodology

The development of MicroLabVR required a structured approach that addressed multiple aspects of the development process. BacArena [13] serves as the foundation for creating simulation datasets used in the VR application. We developed an R-script to convert data generated by BacArena [13] to two CSV files – a population dataset and a substance dataset. For demonstration purposes, the *SIHUMI* dataset has been used. The population dataset contains one organism and its associated attributes per row: *label_of_dataset, time, x-coordinate, y-coordinate, biomass, genotype_ID, phenotype_ID, genus_species_strain, flux_of_metabolite_1, flux_of_metabolite_2, flux_of_metabolite_3, flux_of_metabolite_4, flux_of_metabolite_5, flux_of_metabolite_6*. The following is an example of an *Anaerostipes caccae* bacterium at time 1 in the simulation:

Population, 1, 3, 17, 0.646973, 1, 8, "Anaerostipes_caccae_dsm_14662", 23.1472, -47.9201, 12.0001, -3.1593, 49.9999, -25.2500

The concentration values are represented as matrices, thus spreading over multiple rows, depending on the size of the simulation area. Each row contains the *concentration of substances* for one y-level in the grid, preceded by *label_of_dataset, substance, time, y_level*. A 3×4 simulation area can look like the following:

Substance, "EX_h2o", 3, 1, 0.4738, 0.3827, 0.2301, 0.1284
Substance, "EX_h2o", 3, 2, 0.7142, 0.9914, 0.9051, 0.0593
Substance, "EX_h2o", 3, 3, 0.4176, 0.6723, 0.8465, 0.3088

MicroLabVR is an application based on the Unity game engine [35]. Unity provides a framework and interfaces for developing 2D and 3D games using C# as the scripting language. We designed MicroLabVR primarily as an Android application to run on standalone HMDs like the Meta Quest 3 [36], which we used to debug and test various versions.
Since MicroLabVR can import datasets of varying sizes, evaluating how it performs under increasing data load is essential. VR applications typically require considerable hardware resources, and standalone HMDs are inherently more limited in performance compared to PCs. To identify these performance boundaries, benchmark tests were conducted using a desktop PC with the following technical specifications: A 12th Gen Intel® Core™ i7-12700KF CPU, an NVIDIA GeForce RTX 4070 Ti 12 G GPU, and 32 GB DDR4 RAM.

4 Design Rationale and Implementation of MicroLabVR

MicroLabVR uses Unity's VR tutorial and pre-configured extensions, like the XR Plug-in Management and the XR Interaction Toolkit. Its UI templates are modified to control the application. All organisms are represented as *GameObjects* that were modeled in Blender [37]. They are color-coded by species to distinguish them. Substances are displayed as *Meshes* in 2D and 3D, which Unity generates at runtime. The nodes are raised to a relative height based on their concentration value, creating a landscape of hills and valleys. A *Shader* colors the areas accordingly to improve interpretation (see Figure 2).
The metabolic behavior of the bacteria is represented by a second *Shader*. This *Shader* outlines the *GameObjects* in different colors. A red outline indicates uptake and a green outline indicates production of the selected substance (see Figure 3). This allows users to quickly identify metabolic activity directly within the Petri dish.
We prepared a tutorial to introduce users to the application. The tutorial menu comprises seven slides outlining the essential steps for using the application and visualizing the data.

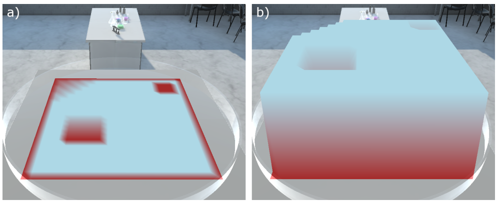

Figure 2. The substance concentration visualized as a 2D heatmap in a) and as a 3D heatmap in b). Red areas represent low concentrations, and light blue represents high concentrations

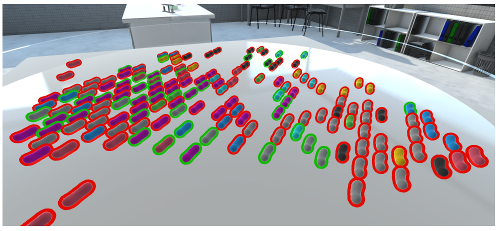

Figure 3. A green outline indicates production, and a red outline indicates uptake of the selected substance

The user can iterate through all slides by pressing the *Button* on the bottom. The tutorial begins with a short welcome and explains how to import the demo dataset. Next, it describes how to iterate through the time steps by moving a *Slider*. Afterward, it elaborates on the utilization of the substance *Toggles* to visualize concentrations and how to switch between the 2D and 3D heatmaps. Finally, the color schemes and flux *Toggles* for visualizing metabolic behavior are explained. The main menu can be operated regardless of whether the user completed the tutorial. Pressing "Use demo dataset" loads the *SIHUMI* demo dataset, and Unity's *Coroutines* read the files asynchronously. Since they distribute the reading process across multiple frames, other methods, like calculating the progress, can run between each frame. This enables the visualization of a progress bar (see Figure 4) that gives the user feedback on the loading status. The datasets are validated to ensure each entry matches the expected format. Feedback is provided based on the specific rule that was violated.

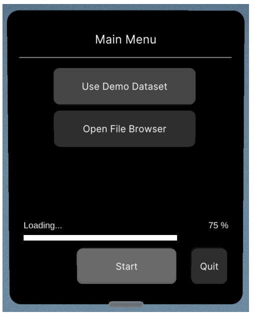

Figure 4. The main menu of MicroLabVR loading a dataset

The main menu shows a successful import message once the script completes the validation without errors. Now, instances of the *Microorganism* and *Substance* classes are created. Another script assigns dataset entries as attributes to these instances. The user can now generate the *GameObjects* by selecting “Start”. A loading bar accompanies this process to provide continuous feedback. After Unity generates the *GameObjects*, the simulation menu appears (see Figure 5), allowing users to control the visualized microbial community within the Petri dish. The user can iterate through each simulation time step by moving the *Slider* or by pressing the “–“ and “+” *Buttons* next to it. Alternatively, the *Buttons* on the left Meta Quest 3 controller can also be used. Compared to simple plots, this enables users to observe how the population evolves over time, including changes in spatial distribution and metabolic activity. This way, dynamic patterns such as growth, competition, or nutrient depletion can be visually tracked and analyzed.

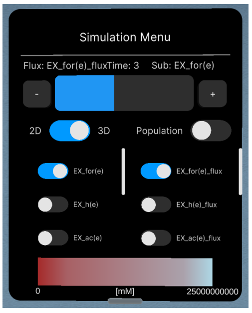

Figure 5. The simulation menu of MicroLabVR, with *Toggles* on the left controlling the substances and the ones on the right controlling the fluxes

The *Toggle* labeled “2D” and “3D” determines the dimension in which the substance concentrations are shown. Each substance can be selected individually via one of the *Toggles* in the left scroll view, with only one active at a time. The *Toggle* “Population” enables users to switch the organism view on or off, allowing them to either focus solely on substance concentrations or overlay both layers to explore potential correlations between microbial presence and concentration patterns. Depending on the user’s visual preference, users can click the color gradient at the bottom to switch between five color schemes for the concentration *Meshes* (see Figure 6).

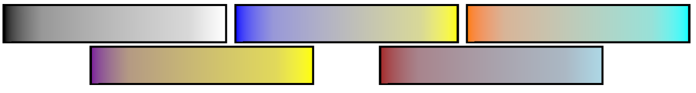

Figure 6. Available color schemes for substance concentration

Lastly, the flux *Toggles* in the right scroll view function in a similar way. Only one metabolic behavior can be shown at once. Organisms are outlined in green when producing the selected substance, and in red when consuming it.
When users hover over an organism, it becomes highlighted. Clicking on an organism causes it to levitate, indicating selection. All available information stored in the attributes of the *Microorganism* instance is displayed in an information panel on the wall. Additionally, a microscopic image of the bacterial species is shown.

5 Performance Evaluation

We created three population datasets of different sizes, as they are the primary factor influencing loading time: D_{Small} with 1389 entries, D_{Medium} with 10600 entries, and D_{Large} with 48000 entries. We evaluated the performance using the Unity profiler, which records the duration of each frame.
While testing, we noticed increased loading times during the import and start of the simulation, which manifested as frame rate drops and temporary screen freezes. The calculated values are documented in Table 1. As expected, the PC-VR setup performed better, meeting the target frame rate of 70 FPS to minimize cybersickness [38] across all datasets. At the same time, the Meta Quest 3 only achieved that goal for D_{Small}. However, both setups experienced frozen screens during the import and start of the simulation, which is unacceptable for a smooth user experience. These results indicate that the standalone Meta Quest 3 is currently limited to smaller datasets (e.g., < 500 *GameObjects*) and the PC-VR version to medium-sized datasets (e.g., ∼ 3000 *GameObjects*) to sustain a stable frame rate above 70 FPS and avoid long loading times or screen freezes.

Table 1. The performance of the Meta Quest 3 and the PC-VR setup while running MicroLabVR: Dimension of the simulation area (*Dim*), number of instantiated *GameObjects* (*n*), time to import the datasets via the Quest 3 ($t_1{}^Q$) and via the computer ($t_1{}^P$), time to instantiate the *GameObjects* via the Quest 3 ($t_2{}^Q$) and the computer ($t_2{}^P$). FPS while the simulation is running on the Quest 3 (FPS^Q) and the PC (FPS^P).

Dim	*Rows*	*n*	$t_1{}^Q$	$t_1{}^P$	$t_2{}^Q$	$t_2{}^P$	FPS^Q	FPS^P
20 × 20	1389	392	0,12 s	0,06 s	0,59 s	0,3 s	71,43	76,92
50 × 50	10600	2500	0,2 s	0,15 s	1,3 s	0,45 s	33,33	76,92
100 × 100	48000	10000	2,2 s	0,9 s	162,7 s	72,9 s	11,21	71,42

6 Discussion

MicroLabVR offers specific advantages over desktop-based microbiome tools, particularly through its 3D visualization in VR. Reinterpreting conventional plot data enables a multilayered and interactive visualization of spatiotemporal microbiome dynamics. It is structured intuitively, paired with a tutorial, guiding users through its functionality. MicroLabVR allows the tracking of organisms in the Petri dish since the *Slider* iterates through the single time steps. Combined with the underlay of substance concentrations, it may help detect microbial behavior, such as migration toward food sources. This remains rather difficult when evaluating graphical plots next to each other, as in BacArena. However, a shortcoming of this is that the user can only visualize one step at a time.
The development faced technical problems. For now, MicroLabVR can only visualize the *SIHUMI* demo dataset since the Meta Quest 3 restricts developer access to its local file system. Implementing cloud integration or using the Storage Access Framework [39] for determined directories could be a workaround. Implementing a file browser in the PC-VR version should be less complicated since there exist some add-ons like the standalone file browser [40].
Users must keep custom datasets within reasonable limits. The spatial dimensions of the virtual Petri dish constrain MicroLabVR's visualization capabilities. If the simulation area becomes too large (> 100 × 100), Unity may no longer render individual organisms correctly, or they may become difficult to distinguish, reducing the clarity and effectiveness of the visualization.

7 Future Work

MicroLabVR offers a solid set of features, although there remains room for improvement. One approach to fully leverage the capabilities of VR would be to visualize 3D layers of a microbiome. This, however, presents a challenge for displaying substance concentrations, as this would require volumetric rather than surface-based representations, necessitating the use of 3D heatmaps for each layer. In addition to these spatial enhancements, the current representation of flux distributions remains limited. Integrating flux directions into the visualization would offer further insight, enabling users to interpret flow gradients within the microbiome better. Furthermore, visualizing exchange reactions would reveal key interaction points and nutrient dependencies between microbial species, critical for understanding community dynamics and metabolic cooperation.

The performance tests showed that MicroLabVR can be optimized for a better user experience. Currently, we use Unity's *Coroutines* to load the data asynchronously. A self-designed approach for asynchronous loading tailored to the application's specific requirements may improve performance. While this may reduce loading times, it would not increase the frame rate. For this, we must reduce the polygon count of all models as it scales with the dataset size.

At the moment, the R converter does not write metabolic fluxes directly into the datasets. This is because BacArena does not clearly map the organisms and their fluxes by itself. This problem must be fixed so the converter can create compatible datasets for MicroLabVR. Direct data exchange via an interface would also automate the process and improve usability. This way, the converter can be replaced entirely.

Regarding the benefits and disadvantages of MicroLabVR, it serves as a proof-of-concept application for extended visualization of microbial data in 3D. While currently unable to fully replace existing desktop tools, MicroLabVR is a solid starting point to design, implement, and test novel interactive visualization techniques for complex microbiome datasets.

To further examine its practical relevance, a valuable next step would be the design of a comparative user study that compares MicroLabVR with traditional 2D visualization tools such as BacArena. Such a study could evaluate interpretation speed, accuracy in identifying spatial or metabolic patterns, and overall user experience across different expertise levels. Although we have not yet carried out this user study, outlining its concept already sets the stage for future validation efforts and could provide important insights into the added value of immersive visualization in microbiome research.

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