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Moliverse: Contextually Embedding the Microcosm into the Universe

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ABSTRACT

We present Moliverse, an integration of the molecular visualization framework VIAMD into the astronomical visualization software OpenSpace, allowing us to bridge the two extreme ends of the scale spectrum to show, for example, the gas composition in a planet's atmosphere or molecular structures in comet trails and can empower the creation of educational exhibitions. For that purpose we do not use a linear scale traversal but break the scale continuity and show molecular simulations as focus in the context of celestial bodies. We demonstrate the application of our concept in two storytelling scenarios and envision the application both for science presentations to lay audiences and for dedicated exploration, potentially also in a molecule-only environment.

1. Introduction

Simulations of molecular dynamics have made great strides forwards in recent years with ever increasing physical accuracy. It is now possible to interactively examine complicated structures and simulate complex processes for proteins and molecules alike. For theoretical chemists a wide array of tools such as *VMD* [19], *Avogadro* [17], *Mercury* [27], *VIAMD* [38], and *SAMSON* [34] exist, but these tools are designed for expert use to support investigation of individual molecules or simulations. While the analysis methods these tools provide are essential to the domain expert, they lack functionality when attempting to show multiple processes simultaneously in the same context.

In recent years, the trend towards confluence of visual exploration and explanation denoted *Exploranation* [45] has gained wide attraction [4, 18, 29, 41]. *Exploranation* is founded on the synergistic coevolution of tools for *exploratory* analysis and tools for *explanatory* analysis. This emerging paradigm shift is built on the realization that the same tools and algorithms that domain experts use to analyze datasets can also be used by the general public to understand the same datasets. Expanding the use-cases of these tools lead to a technological cross-fertilization between domain specific use and science communication, which in turn causes an increased usability that is extremely useful in public outreach activities inside informal science institutions [46]. The use of *Exploranation* in immersive display environments, for example power walls, planetariums, or head-mounted displays, has large potential as they increase the notion of scientific context to the presented datasets. Furthermore, immersive environments also provide the necessary scaffolding of knowledge to the general public, and serve to accelerate scientific discoveries for the domain scientists themselves [10].

So far, the domain expert tools used to analyze molecular dynamics lack many of the features to make them capable of supporting *exploranation*. The work presented here aims to reduce this gap, not by making the domain science tool more *explanation*-capable or the contextualization tool more *exploration*-capable, but rather by embedding the capabilities of one into the other, thus combining the strengths of each tool. In this work, we utilize the *VIAMD* software [38], a feature-rich molecular dynamics analysis tool as the domain expert tool. It is designed to operate on a single screen, but lacks the capability to render in immersive environments on its own. For the

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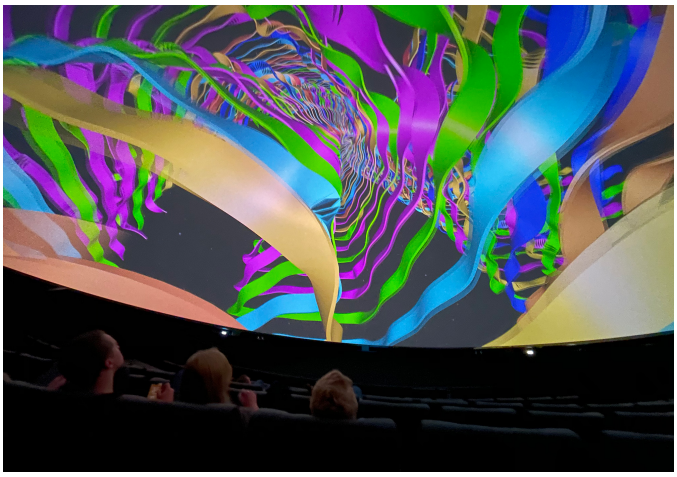


Fig. 1: Moliverse used in an immersive stereoscopic planetarium. The data displayed and being analyzed is a amyloid fibril protein aggregates.

contextualization framework we utilize *OpenSpace* [3], which is designed for displaying a variety of datasets in immersive environments covering vast scales throughout the universe, but lacks the ability to render molecular datasets.

Specifically, our *Moliverse* system allows us to show molecular data in the context of astronomical science shows to audiences in dome theaters worldwide. Our goal with this approach is to make the vast amounts of molecular simulations accessible to the public in their accurate scientific context while simultaneously opening up the benefits of immersive display environments to domain scientists. We present two use cases that highlight this acquired functionality: (a) a molecular composition of planetary atmospheres at different altitudes, complementing the already physically-based rendering inside *OpenSpace* [8] and highlighting the change in composition and density and (b) a series of proteins highlighting the variety of conformations and sizes in the context of a scale ladder of other objects. This last use case is a modern reimagination of a portion of the seminal "Powers of Ten" video by Eames and Eames [9, 32]. The remaining aspects of this video are already present in the *OpenSpace* software.

In summary, *Moliverse* provides us with the capability to:

- render molecular simulations in the context of space, illustrated with the visualization of atmospheric composition of different planets and Titan,
- utilize several display modalities, such as laptops, touch table, planetaria, and head-mounted displays, and
- facilitate the analysis of domain scientists to present their results in an immersive environment.

2. Related Work

Our work addresses and joins three research topics—interactive visualization for science communication, molecular visualization, and navigation across different scales—as we describe next.

2.1. Exploranation

The large availability of scientific datasets and performant computing materials have led some science centers to explore the possibility of providing visitors with the same visualized datasets or models that domain experts use. To facilitate the understanding of these complex datasets by a lay audience, the interactive exploration is augmented by annotations, figures, and general explanations. For this synergy between exploratory systems, usually used by experts, and explanatory visualization that usually guide readers, Ynnerman et al. [18, 45] have coined the term "exploranation." Exploranative systems provide a meaningful pedagogical opportunity when accessing and interacting with challenging scientific concepts that are beyond the comprehension of a non-expert public. Indeed, as they directly explore visualizations of real scientific data, the tailored additional explanations given to them facilitate self-generation and discovery of the communicated concepts. A good illustration of the exploranation concept lies in the *OpenSpace* system [3], which is used by experts and laypeople alike to explore astronomical datasets. Today, the system is versatile enough to allow visitors to explore, alone or guided live by a facilitator such as in a dome-theater, fine-grained and precise images of planetary bodies or data from far-away stars. Beyond the infinitely large, the concept of exploranation has also been used to explore nano-technology, its benefits, and potential pitfalls. For example, the *NanoSim* system [11, 18, 37] relies on Virtual Reality and exploranative concepts to address misconceptions in nano physics. With our own system, we aim to reuse the versatile *OpenSpace* system to visualize molecular datasets and convey molecular concepts to a lay audience via the exploranative concept [25, 42].

The visualization of molecular structures has long been a focus of the visualization community [26], and many different approaches have been developed to date [23, 24]. Today, we are able to visualize even complex structures in real time [6, 28, 39] and are able to produce illustration-quality interactive environments that also bridge the scale-boundary to meso-scale environments [22, 33]. The focus in our own work, however, is not to make advances on the front of molecular visualization but instead to integrate it in much larger-scale environments.

2.2. Navigation and visualization of different scales in context

While merging tiny molecular concepts within the immense scales usually displayed by *OpenSpace* promises to allow us to provide necessary astronomical or astrophysical context to molecular concepts to a general audience, our prototype faces the challenge of having to be able to visualize and navigate data at scales covering more than 20 orders of magnitude (see an overview of the scale range in Figure 2). This issue is particularly well illustrated and solved in Eames and Eames' "Powers of Ten"

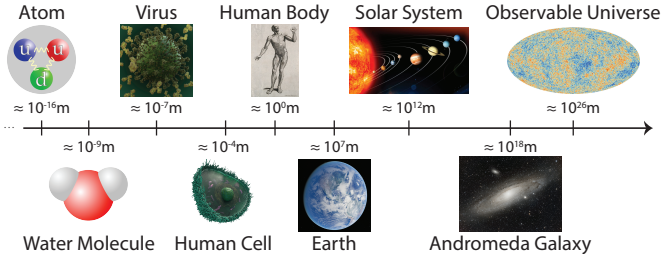


Fig. 2: A scale axis of reference objects presenting the vast scale differences between the molecular world and the observable universe.

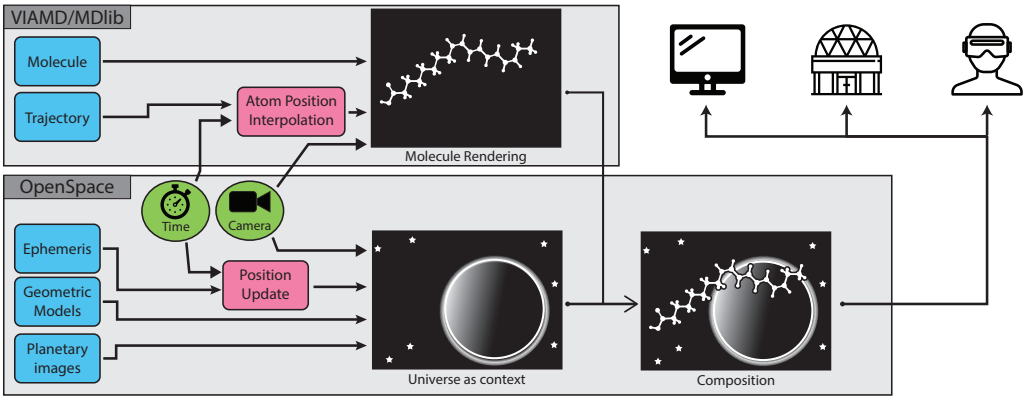


Fig. 3: A schematic display of the integration of the *MDlib* rendering library of *VIAMD* into the *OpenSpace* environment. Each component of the pipeline is rendering its respective datasets individually using the same global simulation time and camera parameters before the resulting output is concatenated and presented to the user.

video [9, 32]. In this video, every 10 seconds, the starting point is perceived from ten times farther out until our own galaxy is visible only as a speck of light. The video uses a step of 10 seconds to gradually provide a zoom out to allow viewers to keep the context allowing them to understand what they see.[1] An interactive version of this idea for data visualization has been realized in various past approaches, for instance by Fu et al. [12] who proposed an innovative two-finger gesture to facilitate the power-of-ten zoom navigation. Another approach was presented by Halladjian et al. [16] who realized transitions between the different representations of neighboring scale levels using their technique of visual embedding. This latter technique was later also adjusted to a spatial control of the scale navigation [15], different from an interactive control. Other approaches have explored, for example, the independent control of several visual abstraction dimensions [44], for instance Mohammed et al. [31] in the context of connectomics and Miao et al. [30] for DNA origami—both of these cases being also examples for the fact that 2D maps of the abstraction spaces, in fact, can be used to control the actual visual representation. In *OpenSpace*, Axelsson et al. [1] implemented seamless transition and rendering between astrophysical bodies at different scales from 25 cm per pixel resolution of the surface maps on Mars to the Milky Way at around 70 MLy per pixel that also support rendering of the microcosm. In our own approach, however, we do not follow the continuous scale exploration exemplified by all of these approaches but keep the astronomical elements and its scale control separate from the molecular scales to avoid having to traverse the huge scale gap between the two. Instead, we use a canvas-like framing to distinguish both parts as we discuss in more detail below.

2.3. Astronomy visualization tools

Apart from *OpenSpace*, there are a plethora of other software tools available to visualize 3D astronomical data sets, the *Uniview* platform [21] is widely used in interactive planetarium shows, as is Evans & Sutherland's *Ditistar* [43], or *Digital Sky* [40]. All of these options, however, have the drawback of being closed-source ecosystems which severely limits the ability to use them for research applications. On the open-source end, *Celestia* [5], *Gaia Sky* [36] and the *CROSSDRIVE* project [13, 35] would have all been potential candidates for an integration with *MDlib*. We chose to focus on *OpenSpace* as it is both the most mature of these options and continuously being updated.

3. Software Ecosystem

To realize our vision of combining the visualization of data at astrophysical scales with molecular visualizations, we rely on a software ecosystem that facilitates the rendering of these vastly different scale levels. We thus first briefly describe both corner stones of our framework, *OpenSpace* and *VIAMD*, before we focus on the implementation challenges we needed to overcome to integrate them with each other in Section 4.

3.1. OpenSpace

OpenSpace is an astro-visualization software able to contextualize vastly different scales from planetary surfaces to galaxies and including the whole observable universe. The universe is navigable in both space and time and users can interactively explore any celestial body. It is built upon an aggregate of many data sources from telescopes, space missions, satellites, and simulations. It is highly extensible and user-customizable with modules and configuration files and acts as an environment enabling the implementation of specific visualization methods, such as the ones presented in this work concerning the molecular world.

The software is employed in many popular science in museums and shows internationally. It is also not only designed for such large-scale installations but targets a variety of devices, ranging from personal laptops, tiled screen displays, and planetarium domes. *OpenSpace* aims at providing freedom of exploration to the public by being immersive and user-friendly, following the principle of Exploranation [45]. To achieve this vision, it can showcase many different visualization sets that can be combined into one coherent scene. Its strength is its extensibility and configurability as it very well adapts to different audiences, mediums, and presentation modes ranging from single users to interactive dome-theater presentations with a

[1] There are also modern and updated revisions of the "Powers of Ten" video such as one by the BBC from 2021 (`youtu.be/2iAytbmXYXE`), albeit this one without the diving into the sub-meter and thus molecular scales.

Fig. 4: A schematic overview of floating point precision error when rendering small objects at large distances from the coordinate system origin in camera space. In this image, 5 significant mantissa bits are used, the coordinate system origin is the center of the orange sphere. Catastrophic cancellation causes objects close to the camera (blue and grey spheres) to suffer from floating point aliasing.

facilitator [42]. Next, we describe our selection of molecular visualization software to be integrated into the framework, before discussing the conceptual challenges from that combination.

3.2. VIAMD and MDlib

VIAMD stands for Visual Interactive Analysis of Molecular Dynamics and is a research tool used to visualize and analyze molecular data [38]. It is designed to integrate both the visualization and the analysis of molecular dynamics in the same environment, while being flexible and interactive. *VIAMD* comprises the *MDlib* back-end library that implements the core features of *VIAMD*. The *MDlib* library is completely independent from the *VIAMD* user interface frontend and hence can be reused by other applications. This makes *MDlib* perfectly suited to process and render molecules in *OpenSpace*. It provides all the heavy-lifting to integrate molecular loading and rendering in any OpenGL context as well as the interpretation of *VIAMD*'s powerful built-in scripting language.

4. Integration of Two Scale-Diverse Visualization Platforms

The integration of these two platforms provides a number of conceptual and technical challenges in respect to the rendering of the comparatively tiny molecular structures within the much larger astronomical context, the transition between and rendering at both visualization targets simultaneously, and the stereoscopic rendering issues that result from the integration. Figure 3 shows an overview of the integration in which the simulation camera and time from *OpenSpace* is utilized in *MDlib* to render the molecules before both images are coalesced into a single output image that combines the two varying scales.

4.1. Rendering molecules at scale

One important technical issue we encountered is the rendering of molecules at the proper scale in space in relation to the other objects. As already noted, there is a very large discrepancy between the scale of a molecule (on the order of Ångströms, 10^{-10} m) and the scale of the whole renderable universe (on the order of 10^{25} m). A system able to represent the entire range of observables from the size of atoms to size of the universe would need to span 35 orders of magnitude (see Figure 2). The traditional approach for rendering, however, assumes a scene that spans only a few orders of magnitudes. Specifically, *OpenSpace* uses the meter for its base unit, which means that celestial objects are specified with very large numbers when rendered, based on their scale and distance relative to the scene graph root. A molecule, in contrast, would deal with tiny values. If not addressed properly, such extreme values thus lead to numerical precision issues due to the way all modern computers approximate real numbers with a finite amount of precision in floating-point arithmetic, following the IEEE 854 standard. Figure 4 shows the effect of this inaccuracy as the gray object is rendered close to the Sun but, due to the relatively high translation from the coordinate system origin, its model-view matrix has been sufficiently effected by catastrophic cancellation, which is visible in the figure as an aliasing effect of the otherwise circular object. In the IEEE 854 standard, a real number value gets mapped to the closest representable floating-point value, but the interval between representable values depends on the number's magnitude: values close to zero are represented with higher absolute precision than the counterpart with a large magnitude. This is an acceptable trade-off for most applications, as larger things tend to have coarser details and vice versa. Axelsson et al. [1] provide a more detailed description of the interval arithmetic and the visual impacts behind this phenomenon.

In our case of molecules in space, certain situations can become problematic. This happens, for example, when resolving local coordinates from each node to the global coordinate system: while rendering, we usually group all transforms in a single model matrix, which can be seen as a function that transforms local coordinates to global coordinates. Similarly, we use a view matrix which transforms global coordinates into view coordinates. If a molecule in its local reference frame has an appropriate numerical precision, that precision will be lost when moving the molecule to its final position in space relative to the root node—the solar system barycenter. The global coordinates, with their lost precision, are then transformed again to the camera view-point, where the molecule may be close to the origin, hence would be able to benefit from great numerical precision, but such precision was lost already. This example demonstrates how one has to be careful when manipulating numerical values in *OpenSpace*. In this case, the problem can be partially solved by pre-multiplying the model and view matrices beforehand. More generally, the issue is circumvented in *OpenSpace* by using double-precision floating-point numbers, but that also comes at a computational cost, and is also generally not used by external libraries like *MDlib*.

There are other issues with the sub-meter scale specific to *OpenSpace*. There are some places in the code where a minimum distance of 1 meters is assumed and changing this would have snowballing implications that would hinder the portability of our prototype with future versions of *OpenSpace*. This is the case, for example, in the camera navigation system, which prevents zooming beyond the 1 meter barrier to prevent precision errors and would therefore completely prevent us from rendering molecules at their correct scale. For these reasons, we decided to represent the molecules at the meter scale (1 Ångström = 1 meter ≈ 1 atom). This setup is, of course, far from optimal because molecules would be the only element in *OpenSpace* ***not*** to be rendered at their correct scale. Nevertheless, rendering molecules at the meter scale does not much impact the resulting

visuals. When looking at an object without context, for example, it is impossible to tell if it is small and close to the camera or large and far away. In our case, looking at a molecule in the void of space typically gives few to no contextual cues to solve that unknown. The few visual cues that are present are either so far or so large that they do not help viewers to relatively assess the size of the molecule. However, beyond software-related correctness, this decision does break the spatial continuity otherwise found in *OpenSpace* or *VIAMD*. We thus need to find ways to ensure that this break in scale continuity is adequately communicated to viewers and users, as we discuss next.

4.2. Transitions between astronomical and molecular scales

The scale discontinuity in particular creates a problem for *OpenSpace*'s ambition to convey a story to audiences about the depicted scientific content. This means that we now require a clear way to communicate the transition between both scales or even visual means to distinguish both scales if we show them simultaneously. In addition, the size of objects at a given scale can only be perceived by viewers through comparison to other elements in the environment. Yet, as we noted above, our environments often lack the visual context and, moreover, neither the astronomical scales nor the molecular scales are environments with which a typical human is familiar. Therefore, the most important concept to get across in this context is the vast scale discontinuity between the molecules and the "regular" subject matter of *OpenSpace*—celestial bodies.

Typically, there are three main factors that affect people's scale perception in a celestial simulation: (a) *travel time*, with a longer time to reach a target meaning that distances are perceived as farther; (b) *salient motion of the visible objects* on the screen, in particular the growth of the target object is an important cue for travel speed as well as the shrinking of any neighboring objects; and (c) *comparison with the environment* as people have some intuition on the scale of, e.g., the Earth or a comet that may share the view with a depicted molecule and can thus be used for comparisons; the International Space Station, for example, looks small compared to the Earth that completely fills the background next to it for any realistic camera setting.

Each of these factors, however, has its limitations. For instance, the travel speed highly depends on the scale at which the camera is operating at any given moment to be effective and non-experts may not necessarily have a reliable understanding of the actual sizes of a given celestial object such as a particular moon of a given planet or the size of a comet, with or without tail. Moreover, the travel time in *OpenSpace* is controlled automatically following an exponential trajectory that depends on the distance to the selected object, so that we can only use the overall scene configuration and the change in an objects' apparent size to communicate scale differences. To do so, we employ a non-linear scaling that depends on the distance from the camera to the molecule. As we get closer to the molecule, it grows bigger—getting further away makes it shrink. We add this effect on top of the natural perspective projection, which makes closer objects appear larger on screen. When navigating towards the molecule, this visual effect thus makes the spectator feel as if the molecule was moving faster towards them and, conversely, it increases the perceived distance from the camera faster than a real object would. When adding a molecular focus in a celestial context we thus ensure a rapid change in visibility and hence communicate the difference in scale to the audience.

To further illustrate the scale difference, we borrow the concept of cut-outs from traditional illustration. Cut-outs are often used to illustrate containment or smaller elements inside another—exactly the same concept we also are trying to communicate. We thus draw an outline around the molecular focus (see Figure 5) to separate its spatial environment from that of the celestial context—inspired both from the concept of Bier et al.'s general *Magic Lenses* [2] and Halladjian et al.'s *visual scale embedding* [16] for DNA visualization as well as related to the squares that were used as a scale measurement or indication in the "Power of Ten" video [9, 32]. The cut-out visual metaphor is well established and allows us to further communicate the scale differences between the molecular focus and the celestial context—the outline indicating this abrupt change in scale.

4.3. Stereoscopic rendering and depth perception

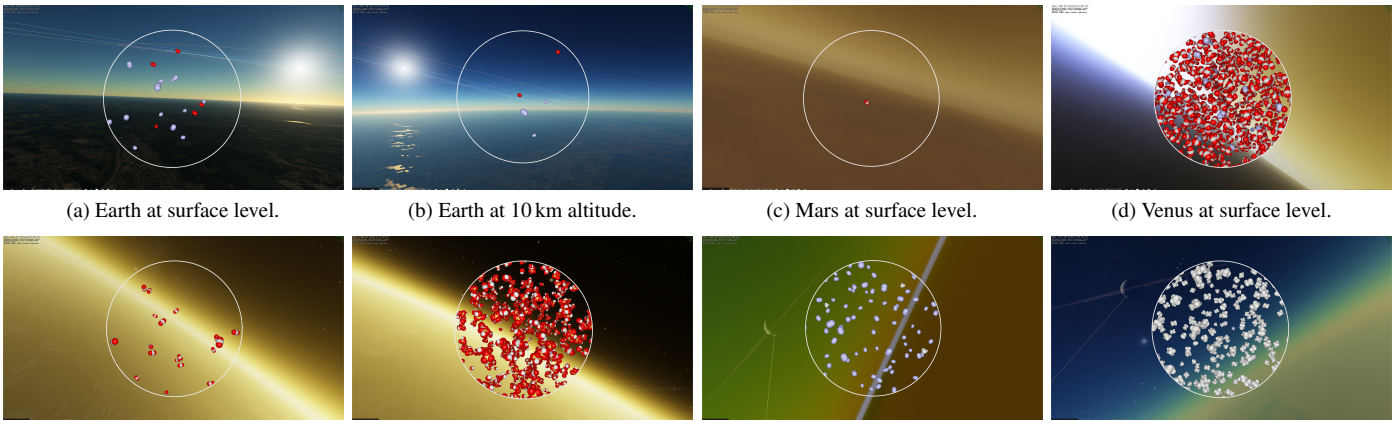
Another challenge is to support stereoscopic rendering at both the celestial and the molecular scale at the same time. In fact, a normal inter-ocular distance (in the order of 5–6 cm) would never allow effective depth perception when viewing planets or larger objects—these would appear as flat objects. In systems like *OpenSpace*, therefore, a much larger virtual inter-ocular distance between the two virtual cameras is used—with the effect that, for example, the Earth, when observed from the distance of few thousand kilometers, appears like stereoscopically rounded ball with a diameter of a few meters. By controlling the ratio of eye separation to object distance a programmer can thus determine the perceived depth of the object in focus.

Most of the time, *OpenSpace* has a single object in focus and the system can therefore automatically adjust the stereoscopic depth to match the size of that object. When navigating from one point of focus to another, the stereoscopic depth is smoothly interpolated. This interpolation of the virtual inter-ocular distance also allows us to transition to a view that depicts the molecular data in correct stereoscopic vision—at the cost that any background celestial objects appear flat in such views.

5. Implementation

We implemented the molecular rendering in *OpenSpace* as an optional module that internally utilizes *MDlib* for molecular loading, processing, and rendering. The module exposes two conceptual types of renderable scene-graph nodes in *OpenSpace* for molecules: `RenderableMolecule` and `RenderableSimulationBox`—one for *out of the box* rendering of molecular systems and one for creating a coarse-level simulation box with rigid-body mechanics (rotation, translation, and elastic collisions) from a set of molecules and their corresponding ratios, respectively. Both renderable types support molecular trajectories as input data. In the case of `RenderableSimulationBox`, however, trajectories represent intra-molecular dynamics.

Each scene-graph node renders into an off-screen frame buffer with its own depth buffer and is later drawn as a billboard within



(a) Earth at surface level. (b) Earth at 10 km altitude. (c) Mars at surface level. (d) Venus at surface level.

(e) Venus at 50 km altitude. (f) Venus with a cloud of sulfuric acid. (g) Titan at surface level. (h) Titan with a cloud of ethane.

Fig. 5: Images of the atmospheric composition at different altitudes for Earth, Mars, Venus, and Titan, taken at a zoom level that suits molecular content. The ring or frame surrounding the molecules serves as an aesthetic highlight for the boundary of the volume in which the molecules are shown and illustrates the scale difference.

OpenSpace. This circumvents numerical precision issues related to large ranges in depth buffers (z-fighting) and facilitates screen-space post-processing. The necessity of such screen-space operations arises from the geometrical complexity of the molecular systems that are comprised of up to hundreds of thousands of atoms. With such levels of geometric detail, a certain level of *visual realism*, for example contact shadows, is required to facilitate spatial understanding under such circumstances.

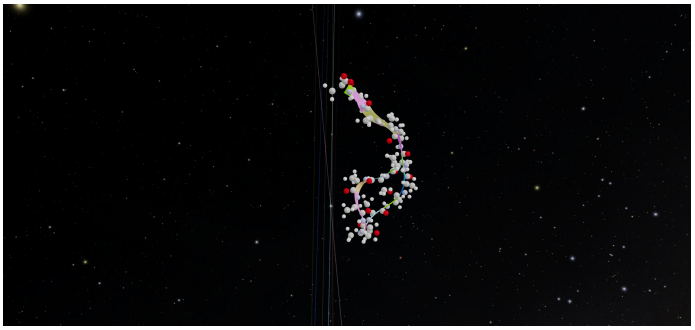
The scene-graph nodes expose properties to control visual representations of the molecular systems as well as a local simulation time, which is loosely coupled to the global time supplied by *OpenSpace*. The local simulation time is progressed by the global time but is wrapped in its local domain. It is ultimately used to control the trajectory frame to be displayed. Molecular trajectories are generally sparsely sampled from their underlying simulation. This imposes discontinuities in atomic coordinates over frames and interpolation is required to reconstruct a *plausible* trajectory. We employ a cubic interpolation scheme that is C^2-continuous and respects the periodic boundaries of the trajectories simulation box. This yields a perceptually smooth motion, which mitigates motion-sickness—an important aspect when targeting large projection surfaces such as domes. The integration of both tools had no significant impact on the performance. With the exception of amyloid fibril dataset, the framerate always exceeds 60 frames per second on a powerful desktop computer.

6. Storytelling

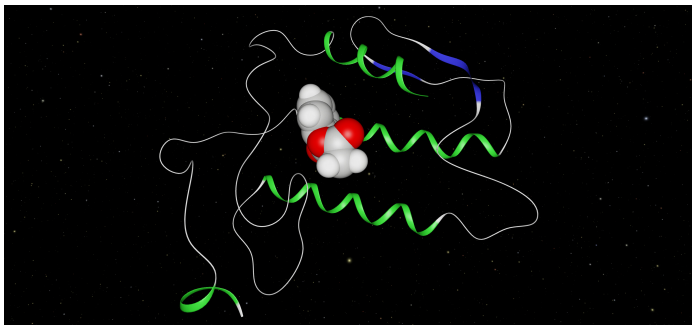
Beyond these technical issues, the following questions arose regarding storytelling: what would be interesting to show to laypeople, how close should we stick to a realistic representation of the data, and how to circumvent the technical limitations or use them to our advantage? We address these questions with the following two examples of storytelling using *Moliverse*.

6.1. Planetary Atmospheres

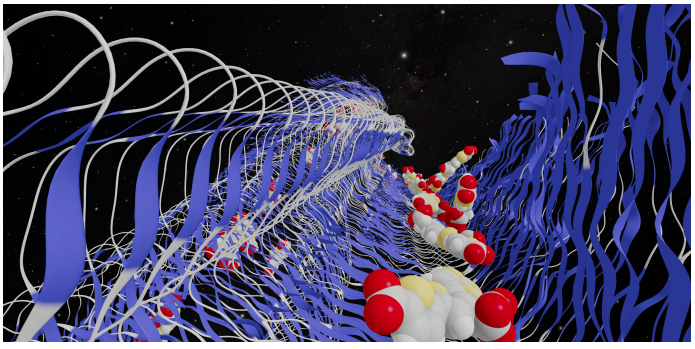
Representing the composition and density of a range of planetary bodies is challenging due to the vast differences in atmospheric pressure. A cubic box of 10 nm size contains, on average, 1, 22, 115, and 919 molecules at the surface of Mars, Earth, Titan, and Venus, respectively. The dimension of the molecular box we want to render thus needs to be chosen accurately to ensure continuity between planets and natural satellites so all boxes could be filled by at least one molecule. Another problem connected to this issue is that molecular species present in traces in an atmosphere could not be represented if we are willing to maintain chemical accuracy of our representation. As described above, we decided to render a simulation box of molecules. For the molecules, we need to distinguish between internal vibration within a molecule, the vibration and movement of atoms within the molecule, and molecular interaction, how the molecule moves and rotates through space and interacts with neighboring molecules. For that reason we built a very coarse simulation, merging the trajectory from a classical molecular dynamics simulation capturing the internal motion of a single molecule with a simple elastic collision model with a circular-shaped collision volume and homogeneous mass to mimic molecular interaction. A box is then filled using known information about the composition and pressure at different altitudes. Figures 5a and 5b show Earth's atmosphere at the surface and at an altitude of 10 km, respectively. The atmosphere of Earth is mainly composed of a mixture of nitrogen (78%) and oxygen (21%) gases as well as a small quantity of argon (1%), water vapor, and other trace gases. As explained before, however, we cannot represent all those molecules considering the low density of our boxes if we want to maintain chemical accuracy. We thus represent only oxygen in red and nitrogen in blue as per CPK convention. These design decisions allow us to show that, at the surface, air molecules take up only 0.1% of the volume they occupy (see Figure 5a) and at 10 km above the surface, the number of molecules is further reduced by a third (see Figure 5b). Mars's atmosphere, in contrast to Earth's, is composed of 95% of carbon dioxide and 3% of nitrogen and is also considerably thinner than Earth's. Consequently, and to maintain coherence and chemical accuracy between our visualizations, there is only one molecule of carbon dioxide in our simulation box (see Figure 5c). Venus' atmosphere is comparable to Mars in its composition (95% of carbon dioxide, 3% of nitrogen, with traces of water and other gases such as sul-



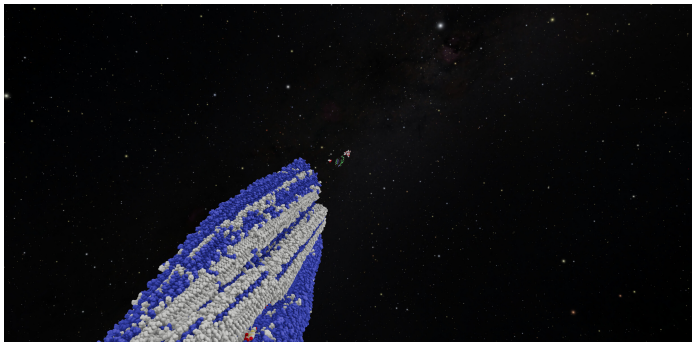
(a) Oligo-alanine chain.



(b) Aspirin molecule in interaction with Phospholipase A2 protein.



(c) Fluorescent markers used for amyloid fibrils detection.



(d) "Looking back" on all shown simulations to highlight the clear size differences.

Fig. 6: Images taken from the molecular exhibit about protein structure of increasing complexity. All molecules are rendered in the same relative context to provide an intuitive insight into their relative sizes utilizing the astronomical background as a subconscious reference frame for the user.

fur dioxide and carbon monoxide) but, in contrast to it, Venus' atmosphere is much denser and the temperature at the surface is close to 500°C, resulting in greater motion in the molecules (see Figure 5d). The atmosphere is so dense that we reach an altitude of 50 km above the surface to find pressure comparable to Earth's surface (see Figure 5e). At this altitude, molecules are excited by the Sun and photochemical reactions on carbon dioxide and traces of water and sulfur dioxide lead to the formation of sulfuric acid that condenses into clouds (see Figure 5f). Titan, the largest moon of Saturn, has an atmosphere composed of nitrogen (94%), methane (5%), and hydrogen (1%). At its surface, the atmospheric pressure is comparable to the one found on Earth's surface (see Figure 5g). At altitudes between 15 and 30 km, the methane molecules condense to form clouds. At this altitude, methane molecules are excited by the Sun's ultraviolet light and react to form ethane molecules that condense at higher altitude around 40 km (see Figure 5h). To illustrate how the transition between the different scenes function, we provide a video as additional material showing us navigating through different simulation boxes around the atmosphere of Titan. This video illustrates how *Moliverse* can be used for storytelling in an immersive environment such as a planetarium by a presenter going on an astro-molecular journey with their audience.

6.2. *Molecular exhibit*

A common practice for domain scientists presenting their results regarding molecular dynamics simulations is to create a video that shows a rendering of a trajectory of a specific molecular system on successive slides of a presentation. *Moliverse* changes this linear and not interactive way of presenting the results of molecular dynamics by taking full advantage of *OpenSpace*'s capabilities of rendering several simulations at different points in space and to use its navigation tool to travel between those different simulations. This form of presentation can be useful to show a progression in the complexity of a system under study, but it also allows the scientists to "look back" to compare the sizes of the different presented simulations to place them in context—both for expert discussions and for presentation of molecular simulations to lay audiences. We utilize the surrounding stars as a background to serve as a continuous reference frame for camera motions around the molecules. Without such background, any motion relative to the molecules would be harder to understand. To illustrate this form of storytelling for scientific data presentation, we provide in the video as additional material, a presentation of three simulations illustrating to a target audience the flexibility of proteins and the resulting large variety of protein structures found in nature. Figure 6 shows stills from this video, starting with a presentation of a simple chain made of 15 alanine residue. Using the rendering functionality of *MDlib*, we change representation to illustrate the necessity of removing single atoms and replacing a chain by ribbons simplifying the view when the number of atoms becomes too large (see Figure 6a). Transitioning to the second simulation, we show the Phospholipase A2 protein to which an Aspirin molecule is binding to deliver its anti-inflammatory effect (see Figure 6b). The color used here illustrates the secondary structure of the protein where alpha-helices are represented in green and beta-sheets in blue. We then show an amyloid fibril found in the brain of patients suffering from Alzheimer's disease. Those structures are caused by misfolded chains that aggregate to form increasingly larger structures that will, in time, impair the normal functioning of the brain. Those structures are largely due to the formation of

beta-sheets illustrated in blue. Approaching the amyloid fibrils, we can see small fluorescent markers used for the detection of those fibrils (see Figure 6c). Lastly, we can "look back" and find that showing all previous simulations enabling the viewer to understand the relative sizes of the presented structures and simulations (see Figure 6d).

7. Discussion

Traditionally, most approaches in molecular visualization [23, 24] focus primarily on various molecule assemblies, typically ranging at most to the size of viruses or cells and their respective molecular composition [16, 33]. While such approaches are excellent to visualize the complex nature of chemical and biological processes, there are also application scenarios that need to depict both very large and very small scales at the same time. In particular, the combination of astronomy with celestial bodies on the one side and molecular information on the other is a fruitful application as molecular configurations or compositions can explain and contextualize many observations at the astronomic level. There is thus added value in finding ways to show both extremes of the scale range in sync, to explain observations to general audiences or to allow scientists to explore respective phenomena interactively and jointly.

As we have shown, this large scale difference poses a number of technical challenges for visualization approaches, such as correctly representing as well as rendering both ends of the scale without artifacts. A traditional continuous scale representation is not possible here, both due to numerical issues in the actual implementation and due to the large difference in scale that would require excessive zooming through irrelevant scale ranges. With our *Moliverse* prototype we instead deliberately break the scale continuity, as it allows us to better show the molecular visualizations in context and to avoid the linear scale traversal. We then make use of linear perspective and non-linear scaling to further allow us to show the molecular data effectively in the context of the celestial scale. We are also inspired by the "language" of traditional illustration and use the concept of explicit cutouts to communicate the scale difference of the molecular data within its context. Taken together, these approaches serve as a new technique within the concept of *Exploranation* [45] that relies on both visual exploration and explanation. In Section 6, we demonstrated the potential of storytelling by showing different scales and subject matter (celestial bodies and molecular structures) simultaneously. Further, we have demonstrated in Section 6.2 that this setup can also serve applications where only molecular representations need to be shown, and we open up the path to displaying such representations to large (lay and expert) audiences in dome theaters.

Nonetheless, numerous questions still remain as we have only started to explore this combination of the opposing ends of the scale spectrum. It is still unclear, e.g., how cutouts should be optimally implemented to maximize people's understanding of the scale discrepancy and to foster exploration—maybe different forms of cut-out are best for either mediated stories (such as in dome theaters) or active exploration of the scientific visualizations. An empirical evaluation of different cutout backgrounds (with/without blur or color), of different shapes (2D circle, 3D sphere), and the importance of previous knowledge of the viewer should be used to determine those that best allow viewers to appreciate the scales. More work on the specific interaction design to allow people to transition between the different contexts and to pull up the additional molecular layers is also needed. Finally, the required detail of the molecular simulations and their realism with respect to pressure and temperature remains unclear, which again may depend on the target audience, the interaction type (mediated watching vs. interactive exploration), and the intended application (shows for lay audiences or tool for scientific exploration and discussion).

8. Conclusion

With *Moliverse* we have combined the two ends of the physical scale spectrum by combining the molecular visualization software *VIAMD* with the astronomy framework *OpenSpace*. This offers audiences the possibility to explore the microcosm in the context of the macroscopic universe. With the launch of the *James Webb Telescope* and the discoveries it will grant the scientific communities in terms of the chemical compositions of exoplanets [14, 20], our work is particularly timely. It constitutes a first step towards building a versatile tool that assists scientists, teachers, and science centers to produce quality scientific communication and mediation by placing past and future chemical discoveries in context.

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