Additional material

The following section (A) contains a description and demonstration of rendering artifacts which appear in two virtual reality APIs. Although the premise of VR SDKs is that your rendering function should not need to be modified, in practice if you are performing some optimizations or advanced graphics in your rendering loop, large artifacts may appear on some platforms. SDKs do not indicate what rendering calls are safe. This is especially problematic because virtual reality requires extremely high framerates, so de-optimizing your rendering is not a possibility. In addition, the artifacts may appear if the user updates their VR drivers, completely outside of the control of the application programmer.

Finally, Section B reviews with a user study how NOMAD VR has improved since the prototype stage into a useful scientific tool already in use in various universities and enterprises.

Section A. Optimization caveats in VR APIs

While often standard OpenGL code can be used within a virtual reality framework to provide an immersive experience, some graphic algorithms make assumptions which are no longer valid in specific virtual reality SDKs due to the post-processing performed by the SDK. We expect that variations these post-processing algorithms will be adopted by other SDKs if they provide advantages in rendering time or quality. Therefore, we recommend avoiding graphic algorithms which interact with them. In particular, we had to discard the point to sphere optimization and adapt the depth peeling algorithms mentioned in the following sections.

We also provide software demonstrating rendering artifacts in virtual reality: we provide a Windows EXE which demonstrates the sphere-disk artifact an android APK which demonstrates the depth peeling artifact. The software can be downloaded from `http://rubengarcia.userweb.mwn.de/CPC2018-AdditionalMaterial.zip`

Section A.1. Point to Sphere

One algorithm to render spheres efficiently uses a point primitive which calculates the sphere radius in screen coordinates in the fragment shader[1].

[1] `https://www.gamedev.net/forums/topic/591110-geometry-shader-point-sprites-to-spheres/`

The spheres may be rendered simply as circles (under the assumption that the user's view plane is parallel to the projection plane or that the spheres are visually small enough). This works quite well in desktop environments, but due to the large field of view in VR, in HTC Vive it shows the spheres as planar discs which rotate in synchrony with the user (Figure A.1, left).

Spheres may be alternatively rendered as elipses [1] . Artifacts appear if the difference between the z component of the sphere origin and that of the eye is smaller than the sphere radius. To avoid this, the near plane distance needs to be larger than the radius of the largest sphere.

In virtual reality devices, the near plane needs to be situated at the glasses position to ensure immersion (otherwise, objects in front of the user will be partially culled); this restriction makes the algorithm unsuitable for virtual reality.

We are using GPU tesselation when available to render spheres efficienctly; however currently few phones support it, so we revert to triangulated spheres (regular polyhedra can also be used if the user requests it, as they are sometimes useful to hightlight the crystal structure).

Section A.1.1. HTC Vive software instructions

Install the HTC Vive drivers, Steam[2] and SteamVR. Drag cytosine.ncfg into NOMADArtifact2.exe. Look left and right to see the atoms behave as rotating disks.

Section A.2. GPU depth peeling algorithms for realistic transparency [2]

This algorithm, when used in VR environments, may compress the left eye to the first quarter of the image, and the right eye to the last quarter, because the VR SDK may set the projection matrices to render each eye to the corresponding half of the framebuffer, while the blending algorithm expects the framebuffer to display only one eye (Figure A.1, right). Again, we expect that most other multiple-pass, render-to-texture algorithms will also have issues when used in VR hardware. However, a simple re-parametrization may be enough for these algorithms to be useful in VR environments.

[2] `http://store.steampowered.com/`

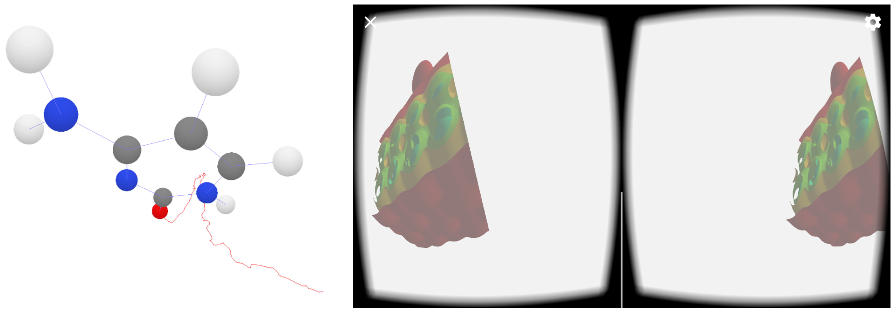


Figure A.1: Left: Rendering spheres as circles looks plausible in desktop environments but results in very visible artifacts in HTC Vive HMD. Right: rendering artifact by interaction between depth peeling algorithm and Google VR SDK result in incorrect image coordinates. See also the software included as additional material.

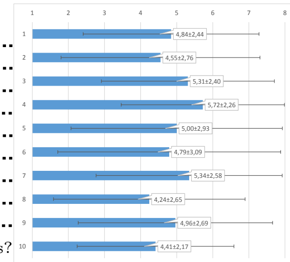
Section A.2.1. Google Cardboard for Android instructions

In order to install the software, enable unknown sources in your device[3]. Install NOMADArtifact1.apk and copy the datasetArtifact1 directory to your phone. Run the app, and open datasetArtifact1/CO2-CaO.ncfg. Move the phone around you to see the rendering artifact.

[3] `https://gs4.gadgethacks.com/forum/enable-unknown-sources-android-install-apps-outside-play-store-0150603/`

Table B.1: Post-Questionnaire

1.I find navigating the VR system easier
2.I find interacting with the VR system easier
3.I find understanding the visualization in the VR system easier
4.I think students will have an easier time understanding concepts by the use of the VR system
5.I think students will find navigating the VR system easier
6.I think students will find interacting with the VR system easier
7.I think students will find understanding the visualization in the VR system easier
8.I prefer the VR system to systems I have used previously for similar tasks
9.In general, do you think the use of VR in this specific example is positive or negative?
10.Can you foresee having an easier time discovering new phenomena by using VR systems like this?



11.Can you think of any study which can be performed more easily on the VR than in classic systems?
12.Can you think of any study which can be performed more easily on the classic systems?
13.Can you think of any additional benefits of the VR representation?
14.Can you think of any additional drawbacks of the VR representation?

Section B. User Study

In the early stages of the project, we used proof-of-concept viewers for specific materials to identify needs and suggestions from final users. This included informal talks with both experts and non-experts at outreach events.

Once enough input was received, further user input consisted of a user study with domain experts, with a post-questionnaire (table B.1) using a 7-point Likert scale and free textual answers. 29 domain experts took part in the user study (a preliminary study with the first 15 participants can be seen in García et al. [3]). We organized two NOMAD Data Workshops, which showed the proofs of concept mentioned in [3] (April 2017) and the current routines (April 2018). We have afterwards participated in various events where the tools were showcased and users were asked to fill the questionnaire: NOMAD Summer 2017[4], LRZ Biology and Life Sciences (BioLab) Summer of Simulation 2017[5], LRZ Molecular Modeling with Schrödinger-Suite Workshop[6]. In addition, final users have shown their datasets in their outreach activities.

We purposely did not test in this study the relative effects of stereo, head tracking and large field of view and of regard, or the differences between CAVE and head mounted displays. It is known that different low-level task types (search, classification, etc) can benefit in various degrees from these effects (see [4] and references within), but complex, high-level tasks require

[4] http://meetings.nomad-coe.eu/nomad-summer-2017/
[5] https://www.lrz.de/services/compute/labs/biolab/
[6] http://www.gauss-centre.eu/SharedDocs/Termine/GAUSS-CENTRE/EN/2017/lrz-molecular-modelling-2017.html

a combination of the low-level tasks, so that in practice all effects should be available. Our objective public is also unable to afford multi-million euro devices, and can only use these in an *opportunistic* manner, e.g. by accessing the services provided by the Leibniz Supercomputing Centre or similar venues. The purpose of the user study is therefore only to confirm objectively that NOMAD VR is a valuable addition to a scientist's toolbox.

Users mentioned the use of Jmol[7], Avogadro[8], Vesta[9], VMD[10], Xcrysden, Paraview, OVITO[11], and POV-Ray[12] for various visualization tasks (depending on the user and the dataset) in their previous, non-VR pipeline. Their VR-included pipeline adds the use of NOMAD VR (plus Paraview if needed for data preparation). In the user study, they compare their original to their VR-enabled pipeline. The fact that various users found the budget to build their own (HTC Vive or Google Cardboard based) installations after testing them at our sites, and their repeated visits at LRZ also speaks for the usefulness of NOMADVR.

With respect to the previous questionnaire, we observe a increase in preference for the VR system in all questions, with an average increase of 0,3 points (from 4,61 to 4,92). All questions except for number 8 are now statistically significant at the 95 % confidence level. While users only express a slight preference for VR, we think that this is due to the fact that NOMAD VR only benefits a small percentage of their whole pipeline. We expect this number to increase as more functionality is added in the future.

Users find the system useful to increase understanding (questions 4, 7, 3). Students (questions 4-7) are expected to find the system especially useful, probably because young people are more used to adapting to new technology.

We have been addressing the comments mentioned in García et al., along with further requests by final users, as detailed in the main text.

Additional answers of question 11 (studies more easily performed in VR) include reaction paths in complex 3D structures, tomography, symmetries of crystals, visualisation of phenomenon involving more than two or three degrees of freedom, dynamic evolution of phenomena like vibrations, compli-

[7] http://jmol.sourceforge.net/

[8] https://avogadro.cc/

[9] http://jp-minerals.org/vesta/en/

[10] http://www.ks.uiuc.edu/Research/vmd/

[11] https://ovito.org/

[12] http://www.povray.org/

cated spatial contour like potential energy surfaces or Fermi surfaces, information visualization, understanding 3D scatter plots, and biomechanics.

With respect to question 12 (studies more easily done in traditional tools), one user mentioned 2D materials.

Further advantages of the VR system (question 13) include explaining research to colleagues and the public, use as a marketing tool, and more advanced story-telling possibilities.

Some additional disadvantages mentioned (question 14) are its perceived qualitative nature (the relatively low-resolution displays in VR are not yet optimal for displaying text).

In addition to the user study, final users have provided us in informal conversations with a list of wishes they would like to see implemented.

- Implement the functionality of established commercial or open source chemistry viewers such as xcrysden and vesta.
- Detect and highlight functional blocks such as methyl groups (-CH_3) or amino groups (-NH_2).
- Add a real-time, low-quality simulation engine to enable interactive changing of the atom positions and other simulation parameters (also, interface with a supercomputer simulation to obtain interactive high-quality simulations)
- Support for specific high-dimensional systems, such as exploration of the landscape of energy values for all positions and orientations (3D+3D=6D) of a molecule interacting with a surface.

We continue the development of the system taking into account the user's feedback and the development of the rest of the NOMAD ecosystem. The user study will also continue gathering users's responses along the lifetime of the software.

Section B.1. Implantation

We have strived to provide our users with software which can adapt to their needs. The Leibniz Supercomputing Centre (LRZ) provides support to Bavarian and associated researchers across their IT needs (computing resources, network, archive and visualization). Researchers are welcome to book the LRZ CAVE and use it for their research, meetings or teachings.

However, portable (PC or phone-based) devices also have their role. Therefore, we support devices such as the HTC Vive or the Oculus Rift (in the PC ecosystem) and the Samsung GearVR or Google Cardboard (in the mobile phone ecosystem).

Various users have indeed bought Vives for their labs after the successful use of NOMAD VR at the LRZ. Other users are using Cardboard glasses for meetings and public awareness events.

The NOMAD VR software is currently already in use in a few organizations: Shell India, Solid-state theory group of the Physics Department of the Humboldt-Universität Berlin, Germany, and Atomically Resolved Dynamics Department of the Max Plank Institute for the Structure and Dynamics of Matter. Hamburg, Germany.

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