Computer Physics Communications 237 (2019) 230–237

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

NOMAD VR: Multiplatform virtual reality viewer for chemistry simulations☆

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ARTICLE INFO

Article history:
Received 16 July 2018
Received in revised form 20 September 2018
Accepted 12 November 2018
Available online 26 November 2018

Keywords:
Graphics
Crystallography
Molecular physics and physical chemistry
Chemistry simulations
Materials science
Virtual reality
Rendering artifacts
Programs associated with the design and analysis of experiments
Advanced computer architecture and special purpose computers on computing in the physical sciences

ABSTRACT

We describe a suite of open source virtual reality programs which can be used to visualize the results of chemical simulations of various types (including access to NOMAD, the largest database of materials science compounds). The programs target virtual reality environments at different price points (M€ CAVE-like[1] systems, commercial products such as the ≈ 500€ HTC Vive, ≈ 100€ Samsung GearVR, to ≈ 10€ Google Cardboards) in order to let final users select the device which best suits their needs. We provide a coherent interface, with graceful degradation of features for less capable devices. Tests with final users in the domains of materials science, theoretical chemistry, biochemistry and biological sciences show that the program can be used to solve certain problems much more easily and intuitively than with previous tools. Users in other fields (fluid dynamics, or climate research) were also interested in adopting the system. Applications to teaching, dissemination, outreach and marketing have also been successful. The system is currently implanted in several universities and enterprises. Additionally, outreach materials in the form of stereoscopic (panoramic) videos can be easily prepared from the viewer's output or the visualization pipeline. We describe the design and implementation of the system, and mention some caveats about using standard graphic optimization techniques in virtual reality environments.

Program summary

Program Title: NOMAD VR
Program Files doi: http://dx.doi.org/10.17632/8n92hc8fbd.1
Licensing provisions: Apache-2.0
Programming language: Mainly C++; interface to Android and IOS in Java and Objective C, respectively
Supplementary material: VR optimization caveats: example of graphic artifacts; NOMAD VR user study.
Nature of problem: Understanding chemical materials and phenomena can be sometimes taxing. Visualization of simulations and exploration using mouse and keyboard interfaces, and the creation of illustrations and videos is helpful, but in some complex cases, it proves insufficient. The use of virtual reality tools allows users of NOMAD VR to enter the simulated world, providing easier interaction and understanding.
Solution method: We have developed a virtual reality viewer for chemistry which has proven useful to help researchers understand their datasets better. Users may either upload their calculations to NOMAD in order to benefit from the centralized environment for data storage and analysis, or prepare their datasets for direct use in NOMAD VR using standard formats such as xyz or Gaussian cube. Workflows for different data types, using open source tools such as Paraview and Meshlab, are also provided. Tutorials for different usecases and a complete description of options can be seen at https://www.nomad-coe.eu/the-project/graphics/virtual-reality-configurator, which also includes a link to the User Manual.
Additional comments including restrictions and unusual features: Download links to pre-compiled software and to the source code can be accessed from https://www.nomad-coe.eu/the-project/graphics/VR-prototype. As final users find additional use-cases and request additional functionality, more features are being implemented. We strive to maintain compatibility with previous builds by adding keywords to the configuration file to enable/disable new functionality. This article documents NOMAD VR as of 23/05/2018 (git commit 65a4204f7b0c6313d6ecd6586dc879ce281b857d).

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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[1] CAVE™ is a trademark of the University of Illinois Board of Trustees. We use the term CAVE to denote both the original system at Illinois and the variants developed by multiple organizations.

https://doi.org/10.1016/j.cpc.2018.11.013
0010-4655/

1. Introduction

We describe in this paper an open-source virtual reality viewer for materials science (NOMAD VR) which can effectively visualize the result of common computer simulations of the evolution of chemical reactions and other interesting data representations used in materials science to evaluate materials properties. The viewer can be used for research, teaching, outreach and marketing purposes.

The next section introduces NOMAD, the umbrella under which NOMAD VR was developed. Within NOMAD, theoretical simulations of materials can be stored; these simulations can be used to study materials properties and to find the best material for a given application. Then, the relevant chemical concepts are introduced in Section 1.2. Section 1.3 covers Virtual reality and related work. The architecture of our system is described in Section 2. Procedures for data preparation are explained in Section 3. Section 4 provides a description of our final system. Then Section 5 provides particularly relevant usecases and spinoffs. Conclusions and future work end the paper.

We also provide additional material which can also serve as a cautionary tale for other researchers who intend to port their software to virtual reality, showing how large rendering artifacts may unexpectedly appear when adding support for new VR APIs. A user study of NOMAD VR, which analyses how final users use the viewers in their work, is also provided.

1.1. Nomad

NOMAD[2] is the largest database of materials science data. It is composed of the following parts: repository, archive, encyclopedia, analytics and advanced graphics, while being supported by high-performance infrastructure. At the lower level sits the Repository, with the collection of input and output files from calculations, and which currently contains more than fifty million open access total-energy calculations (and growing rapidly). The repository data (which supports around 40 *codes*) is transformed into a code-independent view: the Archive. A materials-centric view of the Archive is provided by the Encyclopedia, while big-data analysis of the Archive using artificial intelligence techniques can be performed by users from the Analytics. Advanced Graphics provides both a remote visualization environment and virtual reality datasets and software to study the datasets provided by the archive, encyclopedia and analytics.

1.2. Chemistry concepts

We introduce here the chemistry concepts our software can display.

A crystal is a solid material whose constituents are arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions. A crystal structure lattice consists of a set of atom positions, an origin and three axis vectors. Repetition of the set of atoms by unit translations along the axis vectors will reproduce all the atoms in the crystal.

The Fermi surface is an abstract boundary in reciprocal space (the Fourier transform of the Bravais crystal structure lattice) useful for predicting the thermal, electrical, magnetic, and optical properties of metals, semimetals, and doped semiconductors. The shape of the Fermi surface is derived from the periodicity and symmetry of the crystalline lattice and from the occupation of electronic energy bands.

A chemical reaction is the process which leads to the transformation of chemical substances into another. Adsorption is a chemical reaction in which a molecule becomes stuck to the surface of a solid.

Electron configurations are the basis of chemical properties. The energy of the electrons can be classified in bands which correspond to the mobility of the electrons in the material. The inner bands correspond to inner orbitals, in which the electrons stay near its original atom. The valence bands correspond to chemical bonds between atoms. The conduction bands correspond to higher energy levels, where the electrons can travel in the material. When an electron in the valence band absorbs a photon and jumps to the conduction band, it leaves behind a *hole*. The *hole* acts as a virtual particle, with positive charge. Excitons are bound states of an electron and a hole, and their wave function is six-dimensional (the wave function is a mathematical description of the state of a system).

A large chemical molecule can contain sub-parts which have a chemically-significant meaning. These subsets of atoms are called residues.

1.3. Virtual reality

Virtual reality is a set of techniques which aim to make the user believe he is inside a virtual world. Head mounted displays (HMDs), user tracking, immersive audio and haptics can be used to achieve this, although current systems commonly focus on HMDs. The technology has evolved significantly since its introduction in the 1960s [1], with multiple waves of interest (in the 1980s and 2000s). Multiple high-quality consumer-grade devices have entered the market these last few years, with an exponential growth in the games sector. The use of these devices for scientific [2] and information [3] visualization can provide useful insights on many datasets, for example by allowing users to explore information from the inside-out (in contrast to 2D techniques which give an outside-in view) [4].

1.3.1. Multisystem virtual reality and examples in the materials science and chemistry fields

In order to ease development of virtual reality software, most hardware vendors provide plugins which integrate into the most common game engines (specifically Unity 3D and Unreal). Software companies can then use these plugins to develop virtual reality experiences for multiple devices. Higher level APIs can also be created [5,6]. A GPL framework for Linux and Mac which has been used in materials science is VRUI.[3]

In contrast our framework uses the low-level SDKs directly; otherwise the use of the game engines would require final users of our system to pay development fees to private companies, reducing our target demographic. In contrast to VRUI, we also support phone-based VR to lower cost of entry. Our framework is licensed under Apache 2.0, which allows both open-source and propietary derivatives (unlike the GPL).

Covise[4] is a GPL2+ general system for simulations, post-processing and visualization. It works in CAVEs and Powerwalls but does not have many options for chemistry visualization.

Paraview[5] is a BSD software for scientific visualization. The CAVE version is not very stable and is not maintained by the Paraview team anymore. Vive (v 5.3) and Oculus (v 5.2) versions exist,[6] but the latest version of Paraview does not have VR support.

2 https://www.nomad-coe.eu/.

3 http://idav.ucdavis.edu/~okreylos/ResDev/Vrui/.

4 https://www.hlrs.de/covise/.

5 http://www.paraview.org.

6 https://blog.kitware.com/taking-paraview-into-virtual-reality.

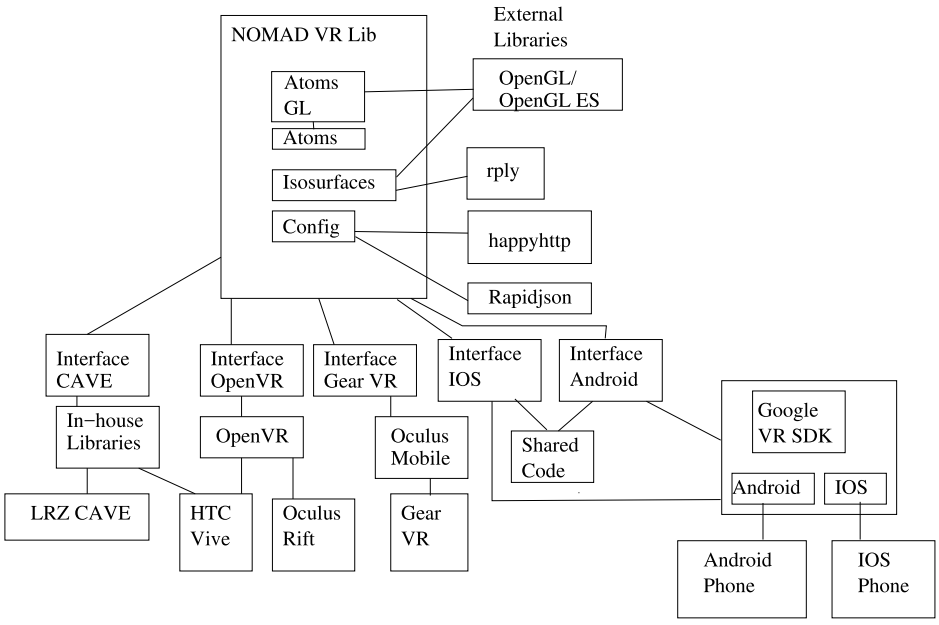


Fig. 1. Block diagram of NOMAD VR showing supporting libraries, SDKs and hardware devices.

Amira[7] is a commercial application for the life sciences with some chemistry support. The VR version works in CAVE and on Powerwall.

Another very complete molecular viewer is Caffeine, which supports CAVEs and previously supported Oculus Rift [7]. The software is available under request, but no license details are publicly available. There are also plans to support new HMDs.

Some researchers target one specific VR platform (e.g. [8]). Haptics interaction has also been explored [9].

VMD[8] is really popular for chemistry visualization. The recent versions can be used with FreeVR or CAVElib, but do not support HMD displays. Other researchers have used VRJuggler.[9] VMD uses the UUIC Open Source License, which does not allow commercial derivatives or redistribution of derivatives using more than 10% of the original non-comment source code.

Nano Simbox iMD [10] provides a free, but closed-source, cloud-based interactive simulator with three exercises: threading methane through a carbon nanotube, changing the screw-sense of an organic helicene molecule and tying a knot in a small 17-ALA protein. An executable for HTC Vive can be downloaded, in addition to non-VR versions for iOS and Android. Desktop versions for PC, MAC will be provided in the future according to its website.

In contrast, NOMAD VR supports a wider range of virtual reality hardware, can be used standalone, and allows users to study their own datasets, or to access the millions of calculations of the NOMAD project, although calculations need to be pre-computed. Early, material-specific viewers exploring various interface concepts were described by [11]. These studies formed the basis of the current NOMAD VR package (an early prototype of NOMAD VR was introduced in [12]).

To the authors' knowledge, NOMAD VR is the only chemistry viewer which supports VR hardware from CAVE to phones, is compatible with both open and closed source derivatives, and is free of charge. Of course, our purpose is not to substitute but to complement the solutions described here.

2. Architecture and software description

Our system uses C++ and the common subset of OpenGL and OpenGL ES to implement the general functionality. To interface with the virtual reality devices, we use Google Virtual Reality SDK[10] (Google Cardboard and clones), Oculus Mobile SDK[11] (Samsung GearVR), OpenVR SDK[12] (HTC Vive and potentially Oculus Rift), and an in-house developed SDK (which supports the CAVE-like[13] environment and Powerwall at the Leibniz Rechenzentrum –LRZ–, and the HTC Vive). Due to the high speed of development of both hardware and software in the virtual reality field, supporting virtual reality hardware using multiple SDKs is advantageous, as it provides redundancy in the case an SDK reaches their end-of-life. Fig. 1 provides a high-level block diagram. Figs. 2 and 5–7 show the different visualizations.

The NOMAD VR Lib contains code to load the configuration files and any additional data required for the visualization. Internally, the information to be displayed is organized as a set of isosurfaces a set of atom positions, and a set of markers. These sets are organized in timesteps (which may be actual timesteps in a simulation or a coherent collection of independent simulations, such as hole positions in an exciton). The atom positions are processed to obtain chemical bonds if so requested. Care was taken to ensure scalability in large datasets (Fig. 2), by using GPU tessellation shaders to display atoms using only one vertex, thereby reducing atomic data storage on the GPU by one to two orders of magnitude. The information is transferred to the GPU for optimal rendering performance. Software forks investigating dynamic loading of datasets (see Section 5.5), as well as Level of Detail (LOD) algorithms (see [11]) are also available.

The different interface modules control how the user may interact with the available information, mapping for example timesteps and isosurfaces to different buttons. The different rendering algorithms are also decided here. If the hardware provides special

7 https://www.fei.com/software/amira-for-life-sciences/.

8 http://www.ks.uiuc.edu/Research/vmd/.

9 https://www.rug.nl/society-business/centre-for-information-technology/research/hpcv/vr_visualisation/mol_visualisation.

10 https://github.com/googlevr/gvr-android-sdk.

11 https://developer.oculus.com/downloads/package/oculus-mobile-sdk/.

12 https://github.com/ValveSoftware/openvr.

13 CAVE™ is a trademark of the University of Illinois Board of Trustees. We use the term CAVE to denote both the original system at Illinois and the variants developed by multiple organizations.

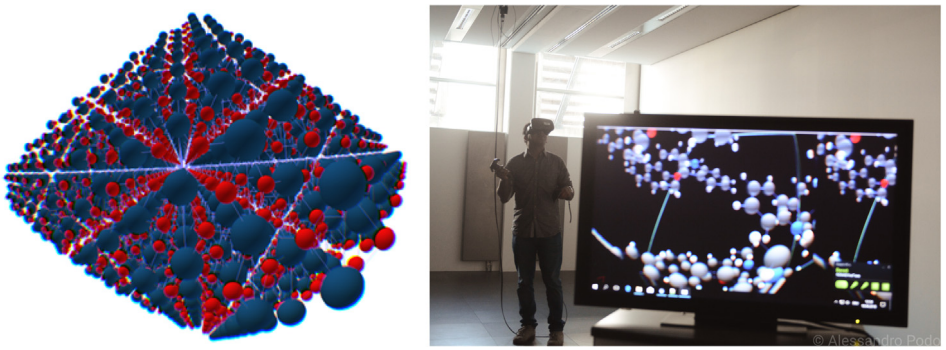


Fig. 2. Iridium oxide nanoparticle (left), and thermal equilibration of Spironapthopyran (SNP) on HTC Vive (right), showing atom bonds.

interaction possibilities, these are also configured. For example, the HTC Vive has primitive haptic support by making the controllers vibrate, which is triggered by our software when users touch atoms.

We considered the creation of a unified API to abstract the VR hardware, but we decided against it because at the moment, the different capabilities in terms of performance, interaction, tracking and visualization would require us to design high-level workflow constructs to express our requirements (for example, *do automatic timestep advance if not enough buttons available*, or *choose this rendering algorithm if performance is high enough and it does not interact with post-processing, otherwise ...*). Instead of embedding a compiler or interpreter (à la UnrealScript[14]), we deemed it more efficient to simply code these in C++ explicitly. This also gives us more leeway and a better understanding of the sometimes unexpected, undesired interactions between rendering and VR postprocessing (see the additional material).

In the case of Google Cardboard, the variety of glasses (some include the possibility of one button press; some do not have buttons; and a bluetooth controller may or may not be available for interaction) forces us to carefully consider how to provide graceful degradation of the interface. We have a continuously advancing time evolution by default. If one button is available, the user may enable/disable movement to explore the scene. If a controller with multiple buttons is available, the functionality to stop/restart the time evolution, advance and return in time and change the active isosurface is exposed, in a similar interface of that of the HTC Vive.

Finally, some support libraries are used to load the 3D models from disk (rply[15]) or to obtain the datasets from the NOMAD website (happyhttp[16], rapidjson[17]). We use small, free, portable libraries to ensure new platforms can be supported easily in the future.

2.1. Dataset selection interface

In PC-based environments, the user can double-click the configuration file, as the ncfg format is opened automatically by our software. Dragging the file into the installed EXE is another possibility.

In the android and IOS environments, we instead chose to open a dialog window to select the ncfg format upon opening the app.

Since GearVR apps start in VR mode by default, we created a companion app to choose the correct ncfg file outside of the VR environment[18], which then calls the GearVR app as a subprocess (or *Activity* in Android parlance).

In the CAVE, the software takes two parameters: the description of the CAVE physical configuration and the ncfg file.

2.2. Adaptations required

The wide range of capabilities forces us to adapt the code to the available hardware: *depth peeling*[19] vs *order-independent, multiplicative blending*[20] for transparency, depending on GPU processing power, *automatic vs manual control of time evolution*, depending on number of available buttons in the interface, *gaze-based vs controller-pointing navigation*, depending on hardware possibilities. The additional material provides some extra detail.

2.3. Domain specific considerations

The (often implicit) assumptions used by domain experts impacts the expectations of final users with respect to the visualization software. This section gives a quick overview of materials-science-specific issues.

2.3.1. Visualization conventions

A chemical simulation uses cells to simplify storage and calculations. The unit cell is a parallelepiped which is defined by three axis vectors a, b, c and a list of atom positions within it. The positions of all the atoms in a crystal can be obtained by repeating the unit cell in space. By convention, atoms at the cell boundaries are repeated in the opposite boundary. The unit cell is also replicated in space for visualization purposes, while the simulation of the atom movements uses periodic-boundary conditions inside the cell.

A supercell is a unit cell which describes the same crystal as a unit cell, but has a larger volume. The axis vectors may also point in different directions as that of the standard unit cell for the crystal, and possibly have a different origin. Excitons calculations are often calculated within the supercell.

The unit cell repetitions, the supercell, the (replicated) atoms colours and sizes, and the electron density should be shown in accordance to non-VR software, including e.g. the expected orientation of the coordinate system (Fig. 3).

2.3.2. Display of trajectories

Chemistry calculations are often periodic in some axes in order to decrease the computational time of the simulations. This means that an atom may *teleport* across the unit cell boundaries. A naïve implementation of trajectories will therefore have spurious horizontal and vertical lines.

However, in most simulations atoms will in general only traverse a very small fraction of the cell size on each timestep, so if

14 https://api.unrealengine.com/udk/Three/UnrealScriptReference.html.
15 http://w3.impa.br/~diego/software/rply/.
16 https://github.com/Zintinio/HappyHTTP.
17 https://github.com/Tencent/rapidjson.
18 https://play.google.com/store/apps/details?id=com.lrz.NOMADGearVRChooser.
19 http://www.nvidia.com/object/Interactive_Order_Transparency.html.
20 http://www.openglsuperbible.com/2013/08/20/is-order-independent-transparency-really-necessary/.

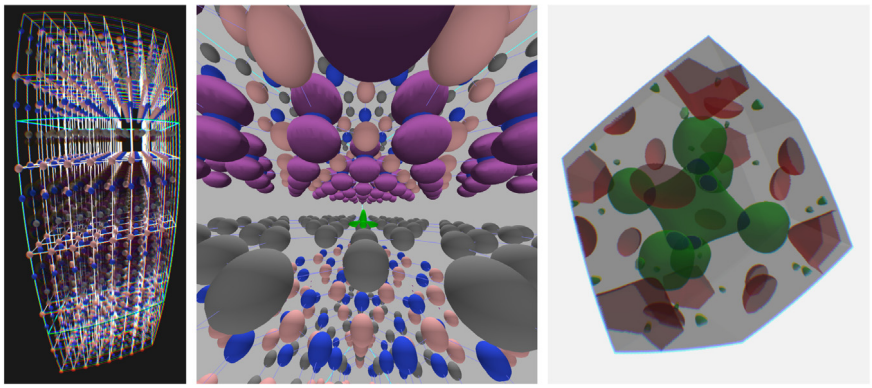


Fig. 3. Left: graphene–Boron nitride (BgC) heterostructure showing unit cell replication (white), supercell (cyan), atoms (grey carbon, blue nitrogen and salmon-colour boron), and electron density (transparent isosurfaces) for a given hole position. Centre: zoom-in showing one isosurface (opaque violet), along with the hole position (green star). Right: Fermi surface of Tungsten (W) from NOMAD Encyclopedia showing Brillouin zone and three bands. The colour aberration artifacts in the left image are a result of HTC Vive preprocessing, and are countered by the device's lenses. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

an atom suddenly traverses more than 90% of the cell size on one timestep, we can be quite sure that the atom crossed the border. The displayed line showing the trajectory of this atom should not include this large (false) displacement. We detect such large displacements and store them as *line restart points* in a per-atom list. At rendering time, the list is used to efficiently display the atom trajectories.

While this algorithm to choose restart points works very well in practice, we are aware that there are some simulations where the assumptions do not hold: high-energy simulation in which atoms are bombarded into a material (e.g. for doping purposes), simulations of impacts from particles which originate from nuclear reactors, or very high temperature simulations.

3. Data preparation

We provide a framework to pre-process the data produced by chemistry simulations into files which can be directly visualized using our software. In particular, volumetric data is transformed into isosurfaces. These files can also be used to create immersive videos for outreach purposes.

Within NOMAD, a collection of Common Gateway Interface (CGI) scripts prepare the NOMAD data corresponding to a given crystal structure or Fermi surface, adding a suitable configuration file for our viewer, and inserting it into a ZIP file which is served to the user. The standardized JSON files used within the NOMAD encyclopedia or analytics themselves to store atomic data can be loaded directly by the VR viewer.

3.1. Input data formats

Materials science uses around forty different codes to perform numeric simulations, although fortunately some standardized formats exist. In particular, *XYZ files* are often used for recording the atom positions in crystal structures or molecular dynamics simulations, and *Gaussian Cube files* are often used for the combination of atomic positions and volumetric data such as electron density. The NOMAD archive can process the input and output files of the codes and provide atomic positions (and in the future electron density and Fermi surfaces) in a normalized format.

Free software and open data formats are used within the NOMAD pipelines. The virtual reality viewer can use user-supplied XYZ or Cube files as a atom position data source, or interact directly with NOMAD. Cube files are pre-processed by our pipeline to extract suitable isosurfaces, as visualization of volumetric data is computationally too expensive for current commodity virtual reality hardware.

The pipeline uses python scripting within paraview to extract VRML isosurfaces from cube files. Atoms may be optionally also extracted similarly if required for the creation of 360° videos. These VRML files are converted into PLY using meshlab.[21] Simplification of the isosurfaces (e.g. for level-of-detail purposes) is also performed by meshlab. The isovalues require domain knowledge and are thus user-supplied. The PLY format was chosen because it is simple and well documented, and small libraries are available to support it in all the platforms we support. In particular rply is an easy-to-use ANSI C library we found useful.

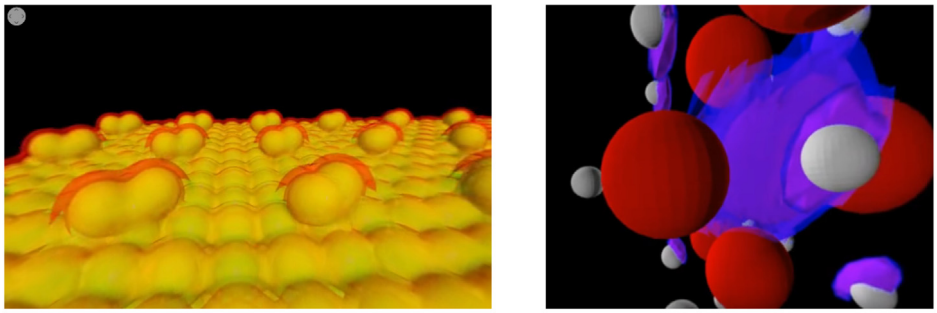
With respect to Fermi surfaces, it is common that the *code* creates a BXSF file, which can be converted to 3D format (single or multiple VRML, X3D or STL files) by the use of chemical visualization software such as xcrysden[22] and visit.[23] We use meshlab again to transform these into PLY files, and optionally to simplify them.

3.2. Use of prepared data for outreach

The virtual reality viewer has the capability of generating (optionally stereo) screenshots of the scene. These screenshots can be used to generate videos, including side-by-side,[24] using e.g. ffmpeg.[25] An SSD is required to maintain a reasonable framerate during screenshot creation. The procedure is described as a step-by-step tutorial at the NOMAD VR webpages[26].

The isosurfaces and atoms produced in the data preparation step can be used to easily create stereoscopic, 360° movies. Our workflow uses blender[27] to create stereo 360° movies (Fig. 4,[28]), as the cycles renderer included within has support for automatically generating images in the correct format. A python script is used to load the ply files corresponding to a given timestep and to set the camera position and orientation. For an in-depth description of the video creation procedure see Garcia [13]. The 360° videos have been shown at the International Supercomputing Conference 2017 and in the Long Night of Science in Berlin, among other events.

21 http://www.meshlab.net/.
22 http://www.xcrysden.org/.
23 https://wci.llnl.gov/simulation/computer-codes/visit/.
24 https://youtu.be/1ytS7n2IIqw .
25 https://www.ffmpeg.org/.
26 https://www.nomad-coe.eu/the-project/graphics/step-by-step-1.
27 https://www.blender.org/.
28 https://youtu.be/XPPDeeP1coM, https://youtu.be/zHlS_8PwYYs.



(a) Adsorption of CO_2 on CaO surface (b) Excitons in LiF

Fig. 4. Example 360° stereo movies created using the VR infrastructure.

Fig. 5. Examples of the virtual reality viewer on GearVR: CO_2 in CaO (left) and AcO_3Sc (right).

4. NOMAD VR

We have developed a material-independent viewer which integrates with NOMAD and can visualize commonly used chemistry datasets. Configuration files (.NCFG) are used to indicate the type of visualization required and the location of the additional files which contain the atomic or electronic information.

The following characteristics have been implemented:

- **Crystal structures and atoms**: Haptic feedback of atomic positions.
- **Molecular dynamics**: Display of atom trajectories and atomic bonds. Possibility of adding new particle types such as molecule residues.
- **Electron densities**: The display of multiple transparent isosurfaces simulates the volumetric electron density within the real-time constraints of VR hardware. These isosurfaces can be optionally shown one at a time.
- **Fermi surfaces**: Including multiple band structure.
- **Excitons**: star-shaped markers can be used to indicate the hole position at each simulation. The simulations can be explored sequentially.

The software starts by reading a text-based configuration file which details what is to be visualized. This includes external xyz, cube or json files for atoms and ply files for isosurfaces. The number of timesteps and the position of markers can also be established. Visualization parameters such as repetitions of the unit cell and instructions on how to render atoms, atomic bonds and supercells can also be indicated. Other parameters focus on the creation of videos: enabling stereo screenshots and controlling the display of controllers and detectors in the HTC Vive. Interaction can be controlled by changing the default speed of the animation and of the user, and by choosing between gaze-based and controller-pointing movement.

After loading the external assets, the user is shown the simulation, and he can use the controllers to fly within. The current timestep, the atoms and the electron density isosurfaces can be chosen by pressing the corresponding buttons. He can also start and stop recording his view for later creation of videos.

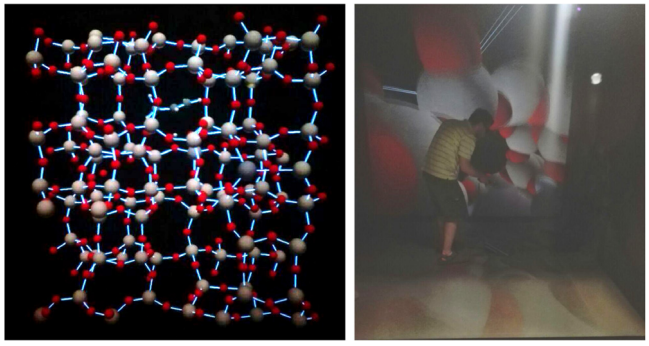


Fig. 6. Different views of DFT-calculated reaction trajectory for the elimination of propene from a Ga-propyl complex in a pore of zeolite. Left: outside view. Right: inside-out exploration.

5. Specific applications and spinoffs

5.1. Nanoparticles

Nanoparticles are composed of a relatively large number of atoms in sometimes-complex crystalline structures. The Wulff construction [14] can be used to generate nanoparticles which can later be simulated in a suitable environment. The use of NOMAD VR can help in verifying that no mistakes were introduced in the particle generation phase, prior to the (much more expensive) simulation phase. Finding these mistakes is sometimes difficult in 2D displays, while in the immersive environment they were detected in a matter of seconds.

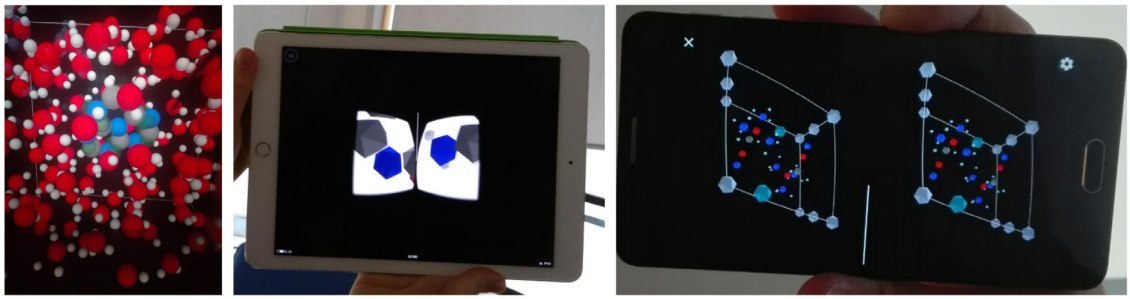


Fig. 7. Left: LRZ CAVE; Heptazine in water showing electron density. Centre: Molecular dynamics simulation of cytosine, on Google Cardboard for IOS. Right: Left: $C_4H_{11}AuBIN_2$ crystal from the NOMAD Encyclopedia, on Google Cardboard for Android.

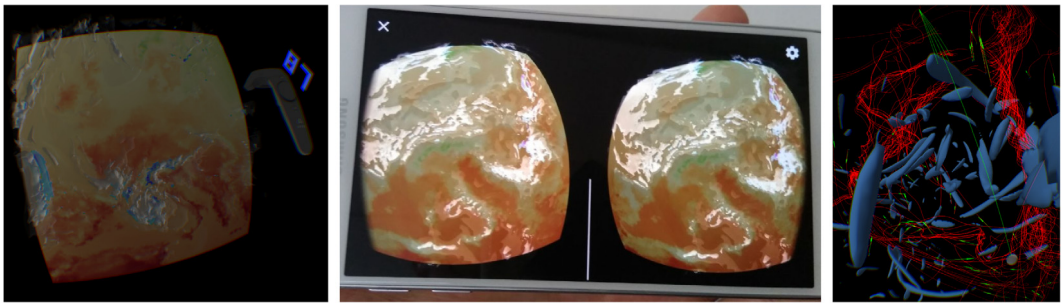


Fig. 8. NOMAD VR on HTC Vive (left) and Google Cardboard (centre) showing the simulated weather over Europe on D. Day and night temperature differences between land and ocean are apparent. Right: Fluid dynamics visualization in HTC Vive.

5.2. Drug design

Drugs can add a variety of chemical groups in order to bind with proteins. When exploring low-energy configurations of these drug–protein complexes, users were surprised of the large amount of empty space between the drug and the protein (minimizing this space produces stronger binding and therefore better drug efficiency). The use of NOMAD VR can help users more easily understand the available space and select the correct ligand for each binding site.

5.3. Inside-out exploration

Section 1.3 mentioned how virtual reality allows inside-out exploration of datasets. Fig. 6 provides one specific example where this is useful in the materials science field. The simulation shows the evolution of propene as it traverses zeolite, which is a porous material.

In virtual reality environments, walking behind the propene gives (according to final users) a better understanding of the simulation. Interestingly, one group of users which was told about the inside-out exploration expressed great interest in the concept but continued exploring the dataset from outside of the zeolite material. It was not until after being physically pushed into the material and behind the propene, that they suddenly recognized the possibilities. The use of the CAVE environment is important in these situations, because the shared physical environment allows us to guide final users within the virtual space.

5.4. ClimEx project

NOMAD VR can be used to visualize general volumetric datasets using the same procedure which is normally used to extract electron density: choose the desired isosurfaces, and either export colour information directly in the 3D mesh, or choose a colour in the configuration file.

For example, we have extracted the simulated weather evolution in Europe in May 1999 (745 timesteps), and displayed surface temperature, precipitation and cloud cover (isosurfaces at 90% and 99% humidity). The data shows a re-analysis climate simulation of the weather pattern over Europe in the month of May 1999, during which the devastating Pentecost flood occurred in the Northern Alpine foothills. (see Fig. 8; the image on the left shows the current timestep 87 – May 4, 1999; 15:00 – above the controller).

5.5. Fluid dynamics

NOMAD VR has been forked in order to create a viewer for fluid dynamics simulations (Fig. 8, right). The software remains NOMAD VR compatible, and adds the functionality to follow a particle. Dynamic loading of isosurfaces has also been implemented in order to support the larger datasets needed in that domain. The software has proven useful in finding particles which show specific behaviour within the fluid; and this information can later be used to create videos highlighting interesting features. Previously, finding such example particles was a complex, time-consuming exercise. Details can be seen at Albert [15].

6. Conclusions

We have presented an open source viewer for materials science datasets resulting from theoretical simulations of chemical systems. The viewer supports multiple VR hardware and can be ported easily to new devices. The software can visualize common formats from chemistry simulations, and it also interfaces to NOMAD, the largest repository for materials science data. Even though the system is still at the prototype stage, various organizations are already using it openly to showcase their work.

We identified specific chemical systems where inside-out exploration of datasets in virtual reality provides tangible benefits: small molecules travelling across porous materials. The free availability of VR software specifically tailored for materials science will help make final users aware of new, better ways to explore and

review their datasets. In addition, tutorials or workshops may be required to make users understand the possibilities.

We have also identified two classes of rendering algorithms and optimizations which interact poorly with the current virtual reality rendering: algorithms which assume the viewing angle distortion to be negligible, and render-to-texture multi-pass algorithms, which clash with SDK post-processing. We recommend other researchers planning to use graphic effects implemented using these techniques to assess the results within VR, and to seek alternative algorithms if artifacts appear. The biggest issue is that, since the post-processing is undocumented and could potentially be changed by an automatic update of the VR SDK, a working program may be inadvertently broken by such an update, with the developers unaware of the problem. We therefore also exhort VR SDK developers to develop API calls to provide information about how the post-processing works, and to formally indicate safe/unsafe rendering algorithms to the application. In-app through overview of the OpenGL state is not possible due to the high cost of state-retrieval commands.

7. Future work

We plan to increase multiuser interaction possibilities by implementing support for network-based shared world between different instances of NOMAD VR (also across different virtual reality hardware). We would like to explore the use of cloud-based services to provide support for high-quality, interactive calculations. Additionally, we are considering the implementation of new features, requested by final users, which can aid in the exploration of certain classes of datasets. In particular, high-energy simulations may require a more intelligent algorithm to display trajectories accurately in the case of periodic boundary conditions. Back-porting of useful spinoff features (such as dynamic loading of isosurfaces) will also be considered. Finally, we are interested in adding support for additional devices and operating systems.

Acknowledgements

The project received funding from the European Union's Horizon 2020 research and innovation program, European Union under grant agreement no. 676580 with The Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence.

Cytosine in Fig. 7 was provided by Raison Dsouza, Max Plank Institute for the Dynamics and Structure of Matter. Photo ©Alessandro Podo/LRZ. The heptazine in water dataset shown in Fig. 7 was provided by Johannes Ehrmaier, while the nanoparticles usecase in Section 5.1 was provided by Jakob Timmermann (both from the Chair for Theoretical Chemistry, Technical University of Munich). The protein-drug usecase in Section 5.2 was provided by Okke Melse (Theoretical Chemical Biology and Protein Modelling Group, Technical University of Munich). The fluid dynamics fork in Section 5.5 was developed by Matthias Albert (Ludwig-Maximilians-Universität).

The climate dataset was provided by the ClimEx project, led by Prof. Ralf Ludwig from the department of Geography of LMU Munich, and funded by the Bavarian State Ministry of the Environment and Consumer Protection, Germany.

Jutta Dreer provided her expertise in CAVE and Powerwall-enabled viewers.

We would also like to thank the anonymous reviewers for their comments

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.cpc.2018.11.013.

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