Virtual Reality toolset for Material Science: NOMAD VR tools

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Abstract

We describe a free-software (Apache 2.0) virtual reality system which provides material scientists with a tool to more easily study simulations of chemical systems at the atomic and molecular levels, and which is compatible with the NOMAD infrastructure (an international, open repository which is developing advanced analysis techniques and contains millions of materials). The system runs on multiple virtual reality hardware, from CAVE-like[a] to phone-based. Informal talks with non-domain experts showed positive responses, and a user study was used to confirm the usefulness of the new system by domain experts.

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

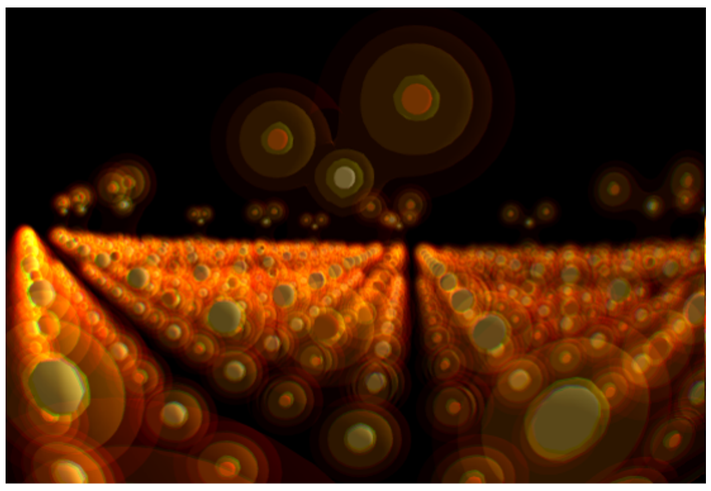

Figure 1: CO_2+CaO(001), full densities (left), 7x7 repetitions using LOD simplification

User Study

15 domain experts were asked to fill the questionnaire in table 1 after using these prototype systems. The new system was in general preferred to current non-VR tools, especially for complex, multidimensional datasets. The results are statistically significant for questions 1,3,4 and 7. An average of questions 1-8 shows a statistically-significant, slight preference for VR. Questions 9-14 provide us with further information about applicability and future directions of work (see paper for details). The data collection is ongoing.

Table 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?

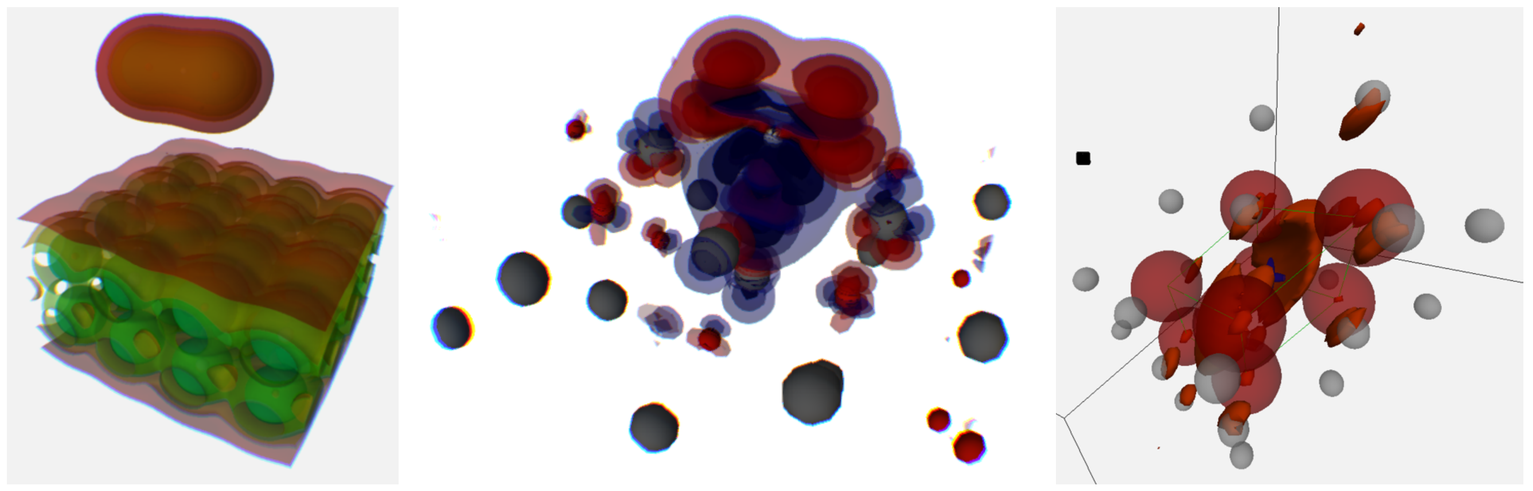

Figure 2: Top: LRZ CAVE-like environment. Bottom: HTC Vive. CO_2+CaO(001), full densities (left), relative densities (center). LiF exciton (right)

NOMAD

The NOMAD repository is an open database of materials, which accepts computer simulations using the most common software packages (called *codes* in the material science parlance). On top of the repository, the center of excellence [1] is preparing an homogeneous and normalized database. Forty *codes* are supported, and development continues. An encyclopaedia allowing complex searches regarding the materials stored is being created. Big data analytics will also allow the discovery of descriptors which can be used to find the best material for a given use case lessening the need for expensive computer simulations of million of chemical compounds. Computations-on-demand are also envisioned. Within this project, advanced graphics (both remote visualization and virtual reality environments) will be used to provide better insights into the materials and their properties.

Adsorption of carbon dioxide on a calcium oxide surface (4D dataset)

This chemical system has important industry applications related to carbon dioxide capture, storage and activation. It is also a prerequisite for further transformation of carbon dioxide into other compounds such as methane.

Excitons in lithium fluoride (6D dataset)

Excitons are bound states of an electron and an electron hole, created when a sufficiently energetic photon interacts with an electron and makes the electron move to a different energy level. They influence the behavior of a material on absorption and emission of light, and are important in opto-electronic (solar cells, lighting), photocathalysis and water splitting.

Developed software

We have targeted Samsung GearVR (smartphone-powered), HTC Vive (PC-powered) and room-sized environments (cluster-powered), so that users can use the system which best suits their needs and budget. Figure 1 shows the Vive system with calcium oxide and additive-blending rendering. The same rendering is used for GearVR. Figure 2 shows both calcium oxide and lithium fluoride on the different platforms, using depth-peeling rendering. We have taken advantage of the SDKs and interfaces available for the different platforms (taking also into account the available processing power), and reused the device-independent code. A live demo of the GearVR software can be checked during the presentation.

Conclusions and future work

The developed tools can be used to study various chemical systems, in combination with classic tools (which users prefer for simple systems). The tools described here can also be successfully used for outreach and teaching purposes. More work needs to be done to increase ease of use, intuitiveness and functionality, but the current prototype is still considered valuable by end users. The current work being performed deals with generalization of these prototypes for external datasets and processing of other chemical data such as crystal structures and Fermi surfaces.

Acknowledgements

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References

[1] NOMAD Center of Excellence. https://www.nomad-coe.eu/ (2015–2017),