The capabilities of virtual reality (VR) have risen dramatically in the past few years in part because of an increase in computing power, but also thanks to the now widespread availability of tools to experience it. Unfortunately, the field of science has been slow to adapt to this change and explore the vast capabilities that VR brings to the table. VR applications have the potential to enhance learning and ease science communication, doing so in an aesthetic manner. This present research aims at filling the gaps by researching and developing immersive visualisations explaining some of the core foundational principles of material science. To this end, multiple examples are presented which show a range of designs as well as interactions between two of the most useful programs for VR applications: Mathematica and Unity. More broadly, this work presents a framework through which other projects are invited to explore the vast possibilities of VR visualisations in material science.

Abstract

The visualisations were developed using the Unity Engine as a visual renderer, and Mathematica to perform the computational calculations. Both communicate together via the Wolfram Kernel with the UnityLink framework built into Mathematica. The interaction between the programs was implemented in three ways:

1. Indirectly through coordinate files (such as .xyz),
2. Using UnityLink functions from Mathematica,
3. Calling the Wolfram Language from the Unity editor.

Framework

**Mathematica**
- Crystalline structure building
- MD simulations
- Chemical database
- Stick and Ball molecule plotting
- Calls to Wolfram Language

**Unity Engine**
- Visual rendering
- Virtual Reality implementation

VR Visualisations

**Molecule Museum**
Immersive exploration of thousands of molecules

Example with caffeine. The keyboard collects user input analysed by Mathematica’s chemical interpreter. Mathematica then sends the plot to Unity.

**Crystal Gallery**
Experiencing the structure of materials

Multiple views of a simple cubic lattice from the inside. The image on the bottom left shows the controls available to the user to navigate the experience. Information is shown for the selected structures, which can be cycled through.

**Diffusion-Temperature**
Feeling the movement of atoms

Top: the interstitial atoms (red) at rest in the lattice (transparent blue).
Bottom: two images at different temperatures, cooler on the left and warmer on the right, showing the range of diffusion.

For more information or a demo, don’t hesitate to contact me at luca.montanelli@bluewin.ch