Interactive Modelling of Molecular Structures

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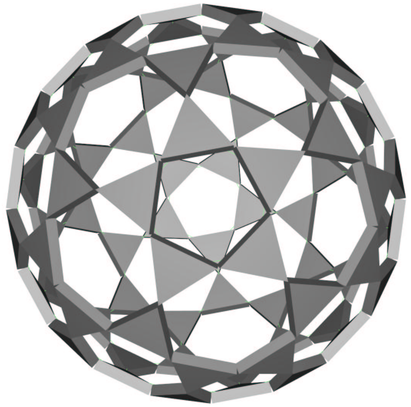


1. Goals

We are developing a visual molecular modelling tool (the "**Nanotech Construction Kit**") to construct, and investigate the structure of, complex molecular arrangements, e. g., fullerenes or silica crystals. This tool could be used to create initial con£gurations for MD simulations, to analyze the results of MD simulations, or to monitor and steer ongoing MD simulations.

2. Approach

We believe that *interactive simulation* is a very powerful approach to molecular modelling. In interactive simulation systems, a user is integrated into a simulation loop by observing the evolution of an MD simulation in real time in an immersive environment, and by directly interacting with individual atoms or larger complexes using six-degree-of-freedom input devices such as wands or data gloves (see Figure 1). A user's manipulations are fed back into the simulation by either adding additional forces to dragged atoms, or by overriding dragged atoms' positions and velocities.

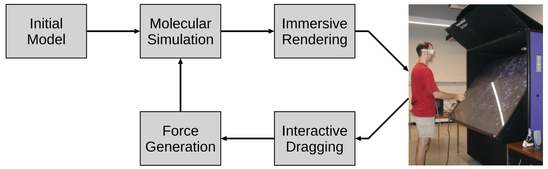


Figure 1: Diagram of the feedback loop of an interactive simulation system. The user is integrated into the loop using head-tracked stereoscopic display and six-degree-of-freedom input devices.

Interactive simulation provides a "virtual sandbox" in which users can experiment with the behavior of large molecules and complexes in a very intuitive way. Our experiments have shown that this "hands-on" approach enables users to quickly create realistic structures (see Section 4).

3. Methods

Our experiments show that immersive visualization is a central component in interactive simulation. Although the Nanotech Construction Kit runs on desktop environments with a mouse and optional additional input devices, it turns out that it is nearly impossible to create structures of any complexity in reasonable amounts of time. The feeling of immersion and the intuitive and direct interaction provided by virtual reality environments are crucial.

Using virtual reality methods imposes two real-time constraints on applications:

- Any movement of the user's head needs to be re¤ected in the display in less than 1/60 s (*display constraint*).
- Any action performed by a user needs to be re¤ected in the display in less than 1/10 s (*update constraint*).

Violating the £rst constraint can lead to dizziness and motion sickness; violating the second constraint can lead to loss of immersion and a feeling of "lagginess."

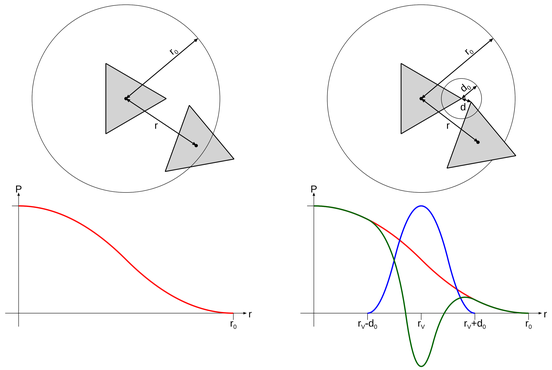


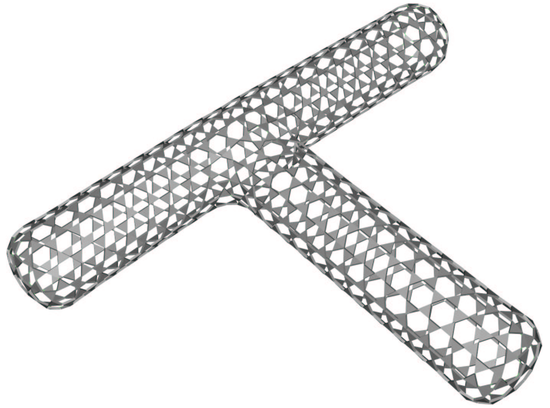
Figure 2: Diagram of the potential £eld used in the Nanotech Construction Kit. Left: Interaction between two non-bonded units (red: repulsion potential). Right: Interaction between two bonded units (red: repulsion potential, blue: bond attraction potential, green: result potential).

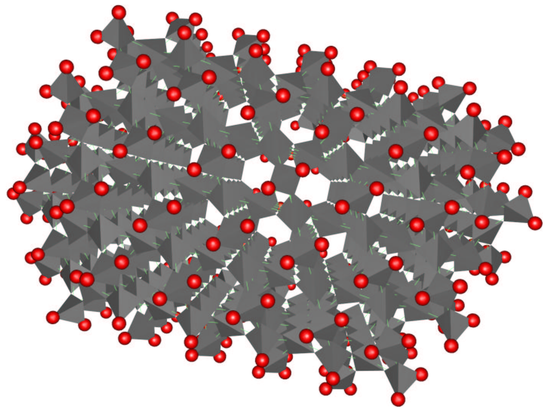
Any immersive application needs to adhere to these real-time constraints. The Nanotech Construction Kit uses the following algorithms to minimize latency:

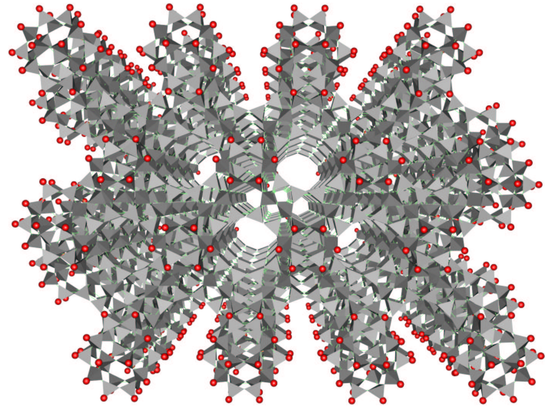
- Geometry-based representation of molecules.
- Simple potential £eld to simulate interactions (see Figure 2).
- Fast £rst-order integration to update atom velocities and positions.
- Geometry-based interaction with override dragging.

These simpli£cations allow us to manipulate large complexes of up to 10,000 atoms on off-the-shelf PC-based graphics workstations. Our experiments show that the simulation is accurate enough to create realistic structures, and more accurate MD simulations can be used to post-process the generated models.

4. Results







5. Conclusions

Our experiments with the Nanotech Construction Kit show it to be an ef£cient tool to assemble complex molecular structures. The provided dragging interaction paradigm is very intuitive, and allows novice users to effectively use the program after a short amount of training. We also learned that the simple underlying simulation method is accurate enough to generate realistic models. It turned out that in order to be ef£cient the program requires a rich immersive environment with at least two six-degree-of-freedom input devices.

6. Future Work

The current version of the Nanotech Construction Kit uses simple rendering and simulation algorithms for real-time manipulation of molecular complexes of up to about 10,000 atoms. Our next goal is to make the program available as a steering framework for large-scale MD simulations involving millions of atoms. To this end, we will develop multiresolution rendering algorithms, and adapt the current simulation algorithm to act as a "prediction method" for a higher-latency MD simulation running on a remote cluster or supercomputer.

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