



Figure 1: The open source glove design (top panels), which we adapted to make application specific VR pinch-sensing gloves (bottom panels)



An open source Etextile VR glove for real-time manipulation of molecular simulations

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ABSTRACT

With VR finding increasing application in scientific research, we are beginning to better understand the domains in which it brings the most benefit, as well as the sorts of gestures which scientific workers find most useful as they navigate simulated virtual spaces. Here we describe an open source Etextile data glove which is designed to facilitate detailed manipulation of 3d objects in VR, enabling scientists to accomplish a range of important molecular research tasks. **The gloves are designed to sense when a user pinches together their thumb and index finger, or thumb and middle finger.** Pinch detection is achieved by closing a circuit bonded onto the gloves using copper fabric. The circuit is connected to an HTC Vive tracker which is attached to the glove via a 3d printed mount that sits on the back of the hand. This design enables us to achieve good positional tracking of the point at which a pinch takes place. Initial tests show that this glove design is **sufficiently accurate and robust to enable scientists to accomplish a range of spatially complicated molecular manipulation tasks** (e.g., tying a knot in a simulated biomolecular protein), **offering a promising alternative to far more costly commercial VR data gloves** which we have found to be unfit for our purposes.

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KEYWORDS

Data gloves; Virtual Reality; Scientific Simulation; etextiles; Open Source

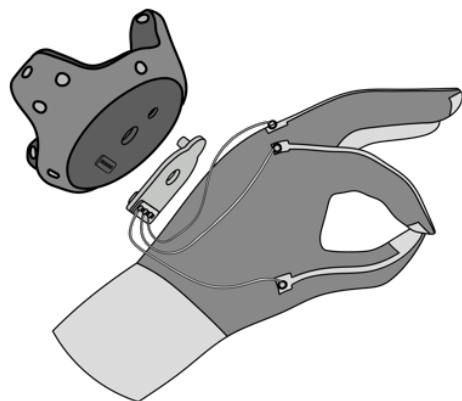


Figure 2: HTC vive tracker attaches to 3d printed mount that houses pogo pins. Pins connect to the copper fabric

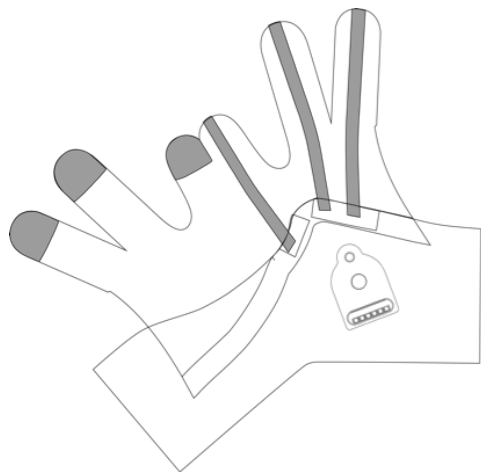


Figure 3: Sewing pattern for the gloves

INTRODUCTION: REAL-TIME MOLECULAR MANIPULATION IN VIRTUAL REALITY

Over the past few years, we have been developing an open-source VR framework which enables multiple participants to move and interact with the structures and dynamics of complex molecular structures and to interact with other users in the same virtual environment. The framework, which we call Narupa [1], utilizes HTC Vive clients which connect to a real-time molecular physics server. To date, this VR framework has found extensive application as a tool for scientific research and education. In a recent study, we compared how quickly scientists were able to accomplish important research tasks using the VR system versus standard 2d interfaces [2]. We found that tasks which required complex manipulation in three dimensions benefitted from VR. For example, when we asked scientists to tie a knot in a small protein molecule, we found accelerations on the order of 10x.

‘FEELING’ THE DYNAMICS OF VIRTUAL OBJECTS

As an increasing number of scientific users have adopted our framework for both research and education, we have noted a number of users reporting that they are able to ‘feel’ differences between different molecular physics simulations, despite the fact that we have yet to implement any form of haptic feedback. Many of the same users who report being able to ‘feel’ the dynamical molecular objects have mentioned the fact that the handheld HTC Vive controllers are actually an encumbrance to their ability to accurately ‘feel’ the simulated objects. Reports like these have inspired us to investigate more direct mechanisms for enabling users to reach out and “touch” simulated molecular objects, without mediation by a controller [3]. From a scientific perspective, it is advantageous to design VR frameworks which enable scientific workers to develop an accurate sense of how a particular molecular object’s dynamics ‘feel’. An accurate ‘feeling’ of a molecule’s dynamical response to external perturbation not only enables a scientific worker to accomplish scientific simulation tasks faster than they would otherwise; it also enhances the researcher’s insight into the system under investigation, allowing them to make more intelligent hypotheses and predictions regarding the dynamics and behavior of a particular molecular system [4].

Given these considerations, we have begun to explore the use of gloves in place of controllers. Using gloves to “touch” virtual objects is a well-explored option [5, 6]. To test the efficacy of gloves in facilitating scientific research workflows, we interfaced the Narupa framework to two different commercial data gloves – the Manus VR glove and the Noitom Hi5 VR glove [7, 8]. These gloves are designed for gestural tracking of hand poses, and distinguishing amongst a variety of potential hand poses (e.g., telling the difference between a ‘thumbs-up’ or a Vulcan ‘live long and prosper’ gesture), for application in environments like motion capture studios. Each glove is equipped with 9-degree of freedom inertial movement units, and bend sensors mounted along the back of each finger. Both of these gloves come equipped with a wrist mount to which an HTC Vive tracker can be attached, enabling absolute positional tracking within the HTC Vive VR system. We have carried out extensive tests evaluating the ability of each of these glove models to enable efficient molecular manipulation, and found their performance not particularly well suited to our purposes for the following reasons: (1) Because these gloves are designed to capture a range of gestures, they require frequent calibration to account for sensitivity to small changes in the sensors as well

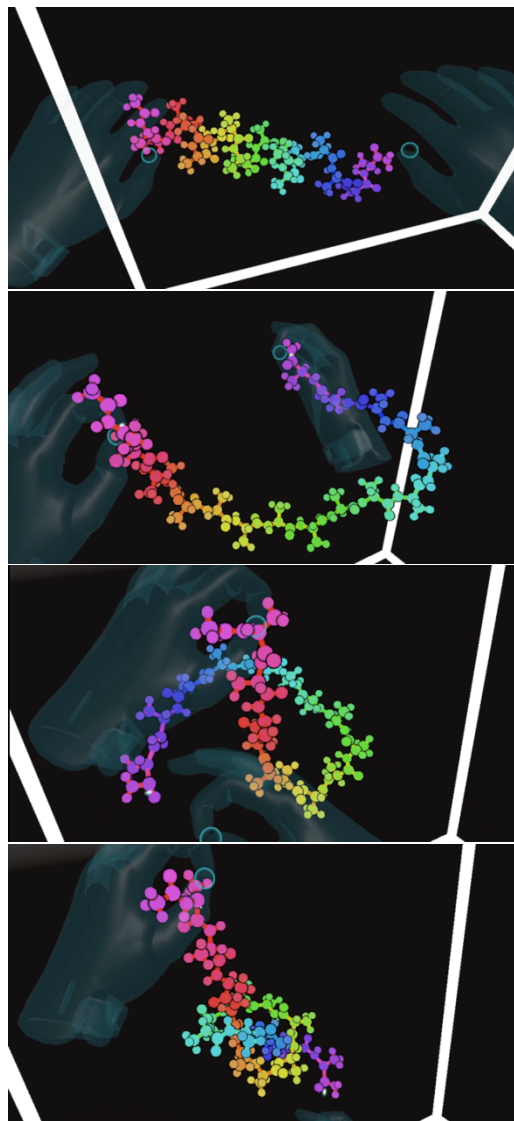


Figure 4: A glove-wearing VR user's first person perspective within Narupa as they tie a knot in a real-time simulation of a poly-alanine protein

as changes to the position of the wrist mounted HTC Vive tracker. For example, calibration is required before and often during each session. This introduces a barrier to usage, for example making it difficult to carry out controlled user studies. Moreover we have found that neither glove is particularly reliable for detecting a pinch between a finger and thumb when a researcher reaches out to 'grasp' a particular atom (or selection of atoms), which an important gesture for the molecular manipulation tasks which we carry out in our laboratory. (2) Both pairs of gloves are expensive (in late 2018, we spent ~\$1.2k on a pair of Noitom Hi5 gloves, and ~\$2.5k on the Manus gloves). Scientific laboratories like our own utilizing the multi-person version of Narupa are unlikely to make such an outlay for non-commodity equipment, especially given the complexity of calibration, their unreliability for pinch detection, and the fact that the Narupa VR framework is often used with 3–4 users, each of whom would then require their own pair of gloves.

APPLICATION SPECIFIC OPEN SOURCE VR GLOVES

As an alternative to the commercial gloves, we took inspiration from recent open-source data glove designs [9, 10, 11], and set out to make low cost open source pinch-sensing gloves that could be used within the VR system for manipulating real-time molecular simulations. The gloves which we designed, shown in Figure 1 and schematized in Figure 2, utilize copper fabric with pogo pins that connect to an HTC Vive tracker mounted on the back of the hand. They have an intentionally simple design which can be reproduced by people with basic sewing skills. The copper is bonded to the fabric using a heat-responsive adhesive, reducing the amount of sewing required, and making the process more accessible to those with limited experience of working with fabric. The gloves are made from stretch fabrics (e.g., lycra) which enables any given glove to fit a range of hand shapes and also permits a larger error tolerance for the glove maker. Figure 2 shows the 3d printed connector which we attached to the glove to make contact with the tracker input pins [12]. The copper fabric is used to construct two circuits which are completed when the thumb contacts either the index finger or the middle finger. When the thumb/index finger circuit is completed, an atomic force is exerted which pulls the nearest atom towards the approximate point at which the pinch occurs. When the thumb/middle finger circuit is completed simultaneously for both the left and right hand, the user can scale the size of the simulation, or rotate its orientation.

Our glove design achieves absolute positional tracking by mounting an HTC Vive Tracker to the back of the hand. The rationale for this design arises from the fact that the spatial location of where a pinch occurs (e.g. between either the thumb and index finger, or the thumb and middle finger) is relatively invariant to a point located on a plane which coincident with the back of the hand. Compared to the wrist mounted HTC Vive trackers used in the commercial gloves, our back-of-the-hand mount has significantly fewer 'moving parts'. As such, it does not require calibration prior to a VR glove session, and we have found it be extremely reliable during VR sessions. Because our VR data gloves directly provide binary inputs for each pinch, they provide little unnecessary data, and require no extraneous hardware. This simplicity allowed us to develop several pairs of data gloves with only basic technical infrastructure, including: a sewing machine, soldering iron, as well as conductive and non-conductive fabrics. Figure 3 shows the pattern we used.

ACKNOWLEDGMENTS

We thank Hannah Perner-Wilson for her work on open-source glove design, Tom Mitchell for guidance and glove-related support, and Helen Deeks for helping out in some initial tests of the gloves. BRG recognizes funding from Arts Council England. AJB is funded through the EPSRC Centre for Doctoral training ‘Theory and Modelling in Chemical Sciences’, under grant EP/L015722/1. MOC acknowledges funding from an EPSRC CASE studentship. LMT acknowledges funding from Arts Council England, the Royal Society, and the Leverhulme Trust. DRG acknowledges funding as a Royal Society Research fellow, Philip Leverhulme fellow, EPSRC programme grant EP/P021123/1, and the London Barbican (Open Lab Funding).

CONCLUSION

Our preliminary tests suggest that this glove design is extremely effective for undertaking complex 3d spatial manipulation tasks in VR like the aforementioned protein knot-tying task, shown in Figure 4 and also at <https://vimeo.com/305823646>. Compared to the commercial gloves, our gloves appear to make the molecular knotting task considerably smoother and less error prone. They require less hardware, no calibration, and one size fits a wider range of hand sizes. In terms of user comfort, the e-textile copper material feels lighter and less cumbersome than the thicker commercial versions. The position of the tracker on the back of the hand minimizes error in hand tracking, enabling more specificity of hand angle and location, and smoother hand motion. Combined, these elements create a more embodied sense of molecular manipulation compared to the hand-held HTC Vive controllers.

FUTURE CONSIDERATIONS

We plan to carry out more extensive controlled user studies to evaluate the extent to which the open-source VR data gloves described herein enable research scientists to carry out complex 3d molecular manipulation tasks like protein-drug binding and protein conformational change. Specifically, we plan to carry out detailed comparisons of our gloves to both the HTC Vive controllers, and to the commercially available glove models. We also plan to evaluate the extent to which glove models like these provide researchers with a better ‘feel’ for the molecular systems with which they are interacting, our intention being that the open source design might offer a robust and viable application-specific alternative to the more complex commercial models.

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