An Immersive Feedback Framework for Scanning Probe Microscopy

Denis Heitkamp[1], Jaccomo Lorenz[1], Maximilian Koall[2], Philipp Rahe[2] and Philipp Lensing[1]
[1]*IuI, Osnabrück University of Applied Sciences, Albrechtstraße, Osnabrück, Germany*
[2]*Physik, University Osnabrück, Osnabrück, Germany*

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Abstract: In this paper we introduce an application for analyzing datasets obtained by scanning probe microscopy (SPM). Datasets obtained by such microscopes are typically depicted by two-dimensional images where the measured quantity (typically forces or electric current) is represented by pixel intensities of a rasterized image. Recording several images of this kind with one parameter being in- or decremented before recording the next image results in three-dimensional datasets. A conventional two-dimensional representation of such data by visualizing an axis-aligned slice cutting through the 3D data seems insufficient, since only a fraction of the available data can be examined at once. To improve the understanding of the measured data we propose utilizing a haptic device with four different real-time haptic models (collision, force, vibration and viscosity) in order to reinterpret nano surfaces in an intuitive way. This intuition is furthermore improved by virtually scaling the nano data to normal sized surfaces perceived through a Head Mounted Display (HMD). This stereoscopic visualization is real-time capable while providing different rendering techniques for 3D (volumetric) and 2D datasets. This combination of appealing real-time rendering in conjunction with a direct haptic feedback creates an immersive experience, which has the potential to improve efficiency while examining SPM data.

1 INTRODUCTION

Scanning Probe Microscopy (SPM) describes a family of techniques that are now well established for the direct imaging of surface-adsorbed atoms, molecules, or molecular structures (Bian et al., 2021). The common characteristic of these techniques is the measurement of a physical quantity in one, two, or three dimensions at the nanoscale, gathered by rasterizing a probing tip along the three spatial coordinates in close proximity to the surface of study. Historically, the scanning tunnelling microscope (STM) was the first invention in the field of SPM: an atomically sharp and conductive tip is positioned with sub-atomic (picometer) precision above a conductive surface of study with a tip-surfaces distance typically in the regime of a few Ångstrom (Binnig et al., 1982). Due to the close proximity, a tunnelling current between tip and sample can be measured if a bias voltage is applied. Systematic measurements of this tunnelling current with respect to the vertical coordinate Z allows the measurement of physical parameters such as the work function, while 2D-mapping along the two lateral positions X, Y delivers images of the electrical conductivity. A fourth data dimension, given by the sample bias, delivers most important information on the electronic and vibrational properties of the sample of study (Stipe et al., 1998). The second key SPM technique is the so-called atomic force microscope (AFM) (Binnig et al., 1986), in particular the non-contact (NC) variant (Albrecht et al., 1991) that can deliver submolecular resolution (Gross et al., 2018). This technique is based on a measurement of interaction forces between tip and sample, thus, it can also be used for the study of isolator materials. In addition to the imaging capabilities, AFM can inherently quantify nanoscale forces at the atomic scale (Heile et al., 2021).

From a data science perspective, SPM techniques can deliver data with three and more dimensions: Spectroscopy (1D), image (2D), or volume data (3D) are among the most common data types. While 1D and 2D data can be visualised with conventional non-stereoscopical projection techniques, the examination of 3D volume data proves to be particularly unintuitive and incomplete. A common method is to investigate only 2D sections from the 3D dataset, which are received by clipping the sets along their principal axes (X, Y, Z). Therefore, it is almost impossible to understand the dataset in context. Another problem is

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the level of abstraction. Datasets obtained by SPM often represent a surface of a few nanometers (Giessibl et al., 2000); yet, there is no natural interaction concept for surfaces of that size for volume data inspection. Last, it is very important to note that SPM image (2D) data are commonly represented in colour-coded form: a user-defined range of the physical measurement values is mapped to a colour gradient and represented in pixel-wise form, which offers the human eye an impression of the different physical properties. Still, further human senses could be involved in the data inspection in order to increase the data accessibility.

Our system contributes an enhanced visual representation and direct haptic evaluation of recorded datasets to the SPM-domain, while also supporting Virtual Reality (VR). Thus creating an immersive experience and a previously unexplored possibility of intuitive data analysis. To achieve this, the data is virtually scaled to many times its real size. This enables natural interaction and investigation in the virtual environment (VE). Our real-time application utilizes the Unity Engine. As a haptic feedback device we suggest the 3D Systems Touch X (Touch X). The device offers a workspace of 160 x 120 x 120 mm and a maximum exertable force of 7.9 newton (N) (3D Systems, 2022). Due to the size of the workspace, our application uses additional input devices to move and scale the representation of the dataset in the VE. Our setup uses a hall effect joystick and motion controller for this, but other devices are also possible for these tasks. Figure 1 shows our experimental setup.

As head-mounted display (HMD) we use a Valve Index with Index controllers as motion controllers. The HMD and the motion controllers use the Lighthouse tracking system, a marker-based inside-out system. The advantage of this tracking over other systems is that it is an open system and additional devices can be added via so-called trackers (Taffanel et al., 2021).

In summary our approach includes the following contributions:

1. A proposal for a new framework in order to present SPM data in an interactive immersive multi-input environment.
2. Four different haptic models for intuitive haptic feedback of SPM data.
3. A real-time rendering framework for stereoscopic data visualization for both 2D and volumetric data.

The paper is organized as follows. After the introduction there is a summary of related work, divided into work on general haptic feedback and work in the field of SPM. Section 3 gives an overview of the entire system, including the actual application, the individual subsystems and components. Followed by a brief overview of the visualization types supported by our application. Thereafter in section 5 we focus on the haptic feedback. The section covers different feedback models for image and volume data. This is preceded by a summary of the interaction concepts. Lastly, we conclude and provide an overview of future enhancements of our system in section 7.

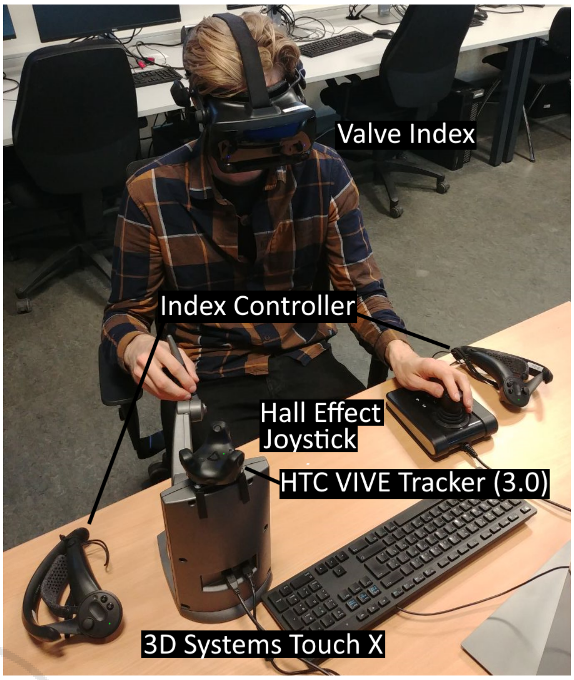

Figure 1: A photograph of our setup. Showing the Valve Index, the Index controllers, the hall effect joystick and the 3D Systems Touch X with an HTC VIVE Tracker (3.0).

2 RELATED WORK

The use of force feedback devices to augment visual data with tactile feedback is a broad area of research. Therefore, we divide the related work into approaches that introduce techniques for haptic reinterpretation of general datasets and then focus on work in the SPM domain.

Burdea (Burdea, 1999) studied the possibilities of haptic feedback for VR in 1999 and Maclean (Maclean, 2000) investigated the best usage of haptic feedback in interactive applications. In 2007 Huang et al. (Huang et al., 2007) explored the utilization of haptic and visual feedback in a simple object manipulation task. The authors used a VE and the participants performed far better when haptic feedback was available. The usage of haptic feedback in VR in order to enhance user performance in the domain of the manufacturing industry was subject of the work of Abdul Aziz and Mousavi (Abdul Aziz and Mousavi, 2009). An interactive device was introduced by Siu et al. (Siu et al., 2017). They created a mobile tabletop shape display for tangible and haptic interaction in 2017. The display is called shapeShift and has a 7 mm resolution. It can show moving objects and provide both vertical and lateral kinesthetic feedback. They also introduced a use case to explore volumetric datasets. Steed et al. (Steed et al., 2021) created a prototype of a mechatronic shape display based on auxetic materials in 2021. Their implementation uses nine actuators on a 220 mm square section of material. The fabric bends in multiple directions, creating a surface which feels smooth and rigid to the touch.

In 2003, Rubio-Sierra et al. (Rubio-Sierra et al., 2003) introduced a haptic feedback interface with a force feedback joystick for an AFM nanomanipulator. The joystick controls the position of the AFM probe with nanometer accuracy and it provides the user with real-time feedback for the interaction between tip and sample. Ladjal et al. (Ladjal et al., 2009) developed a realistic visual and haptic feedback simulator for real-time cell indentation in 2012. They used the Phantom Omni (now 3D Systems Touch) as haptic input device. Another interesting approach with the Touch X (formerly Geomagic Touch X) was introduced by Alabdulmuhsin (Alabdulmuhsin, 2015) in 2015, he published a thesis about a force feedback haptic interface for AFM.

Unlike the aforementioned work, our application works with previously scanned data instead of directly controlling the SPM. Furthermore, in addition to the haptic feedback, the data is displayed using the common and widely accepted Unity Engine, which improves the expandability of our approach.

3 SYSTEM OVERVIEW

Our system consists of four major parts: (1) the actual application, (2) the SPM data used, (3) the haptic device and (4) additional human interface devices (HID). Figure 2 provides an overview of the components and the interfaces between them. The application processes Unity 2D or 3D Assets, data from the haptic device, and inputs from other devices. After processing the current data from the haptic device and the additional HIDs, the force magnitude and direction is sent to the haptic device (in our case the Touch X and addional HID in form of a hall effect joystick and motion controller).

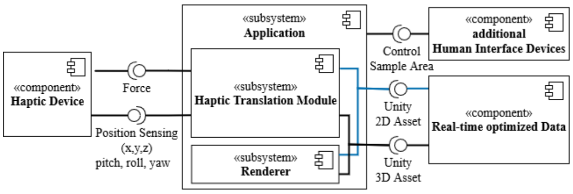

Figure 2: System component diagram.

3.1 Unity Assets

Using the SPM, a sample is scanned and saved either as an image or volume dataset. A Python or Matlab script may be used to transfer the datasets to the so-called Gwyddion file format. Gwyddion is an open-source software with its native file format (Nečas and Klapetek, 2012). Since the software is very common among SPM scientists, our application supports the import of Gwyddion files for visualization and haptic purposes, while wrapping a C library that is part of the Gwyddion project. Afterwards, the files are saved in a native Unity format, so that they can be used in real-time. Figure 3 shows the entire process from data obtained by SPM to real-time capable Unity Engine assets.

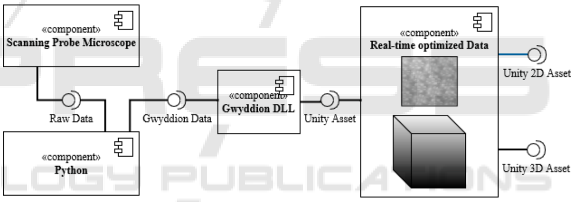

Figure 3: Import workflow component diagram.

3.2 Real-Time Application

The application subsystem is illustrated in Figure 4. It can be devided in two main components, the renderer and the Haptic Translation Module (HTM). The renderer is responsible for the visualization of the Unity assets. Our HTM calculates and transmits the force to the haptic device based on the current inputs, the selected feedback model, and Unity asset. Thus both components require a certain Unity asset. In addition to these components, there are other modules that also manage e. g. input, sound, and physic, but we stay in focus on the renderer and the HTM, since these make the contribution for this paper.

3.3 Haptic Translation Module (HTM)

A component-based overview of our HTM is depicted in Figure 4. The virtual probe position of the haptic device is used in relation to the position of the virtual data representation within the application to cal-

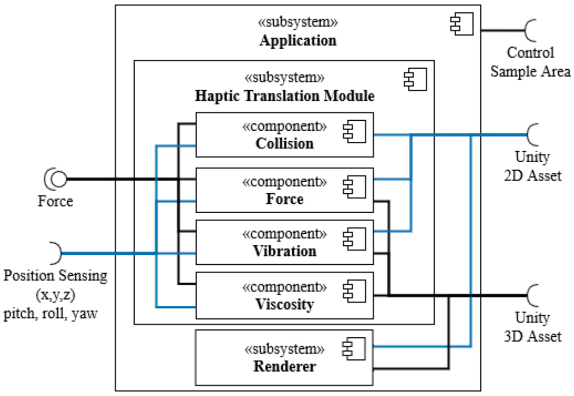

Figure 4: Application component diagram.

culate intensity and other parameters for the respective feedback model. For this purpose, it is necessary to obtain the probe position of the haptic device and to send the parameters to the device. Depending on whether image or volume data is analyzed, different haptic models are available, thus the feedback components require a corresponding Unity 2D or 3D asset. In addition, the components depend on data from the haptic device. Each feedback component offers a force magnitude and direction based on the actual inputs and the loaded Unity asset.

3.4 Renderer

In addition to haptic feedback, the data is also displayed in the VE for orientation and visual examination. The application utilizes Unity's Built-in Render Pipeline.

To render something in Unity, it is necessary to provide information that describe the shape and the appearance of the surface. Meshes are used to describe shapes, and materials are used to describe the appearance. Materials always refer to a shader object. Shaders perform calculations that determine the color of pixels on the screen.

Unity does not inherently provide shaders suitable for displaying SPM datasets. Therefore, we had to develop our own shaders.

4 VISUALIZATION

We implemented different visualization variants for image and volume data, which are described in detail below.

4.1 2 D SPM Data

The usual way to present a 2D SPM dataset in an application is as a colored image. The data is normalized and rendered via separate transfer functions for RGB and alpha (Ljung et al., 2016), The process is illustrated in Figure 5.

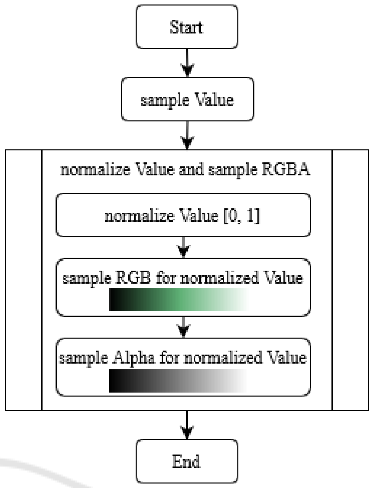

Figure 5: The process to render image datasets.

However, there is an alternative way of visualization which utilizes a displacement mapping technique to visualize the image data as a terrain (Karhu, 2002). Interpreting the data as a height profile enhances the analysis of the data in 3D and benefits especially from the stereoscopic display. Figure 6 presents both visualizations of an image dataset.

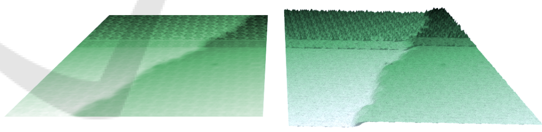

Figure 6: Image data comparison between flat (left) and terrain representation (right). With transfer function Olive for RGB. The used dataset is PTCDA on Ag(111).

4.2 3 D SPM Data

In our application, the volume data is represented as cuboids (Weiss and Navab, 2021). The aspect ratio of the cuboid corresponds to the aspect ratio of the actual data. The visualization uses a ray marching method. Our adaption of the ray marching technique includes the comparison of the value with a threshold and is shown in Figure 7.

This is the common technique for volume rendering (Galin et al., 2020). The method is based on Hart's sphere tracing, published in 1995 (Hart, 1995) and Drebin et al.'s Volume Rendering pub-

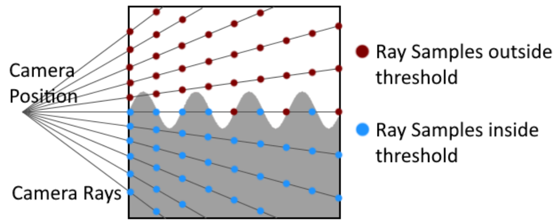

Figure 7: Ray Marching for SPM data with threshold.

lished in 1998 (Drebin et al., 1988). Ray Marching demands more computational power than common rasterization-based rendering techniques, since its performance is heavily related to the virtual camera resolution. Also it is dependent on the camera position. In VR, two cameras are used, each rendering a high-resolution image for the respective eye. This makes the technique particularly expensive for VR applications, and correspondingly powerful hardware is required.

As with image data, the data is then normalized and rendered using transfer functions. The complete rendering process is shown in Figure 8.

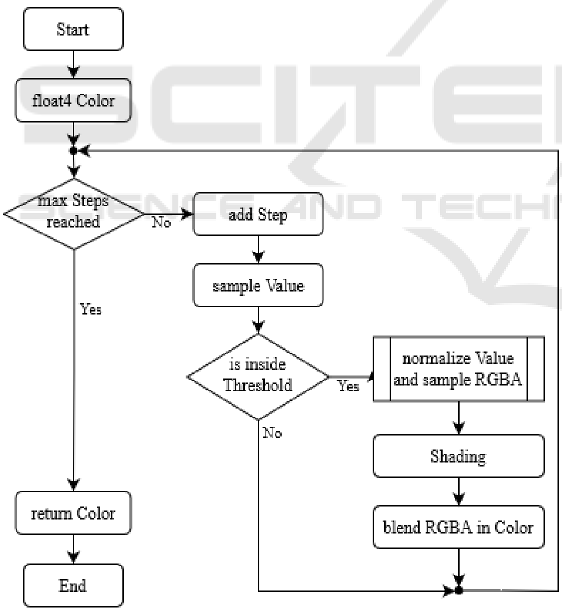

Figure 8: The process to render volumetric datasets.

Figure 9 presents a rendered volume dataset using ray marching with and without a threshold value and applied transfer functions.

In addition to the threshold representation, we have created further visualizations to analyze the volume data. One visualization variant is an extension of the threshold value, where only data representing a certain value is visualized, resulting in visualization of an isosurface. The visualization linearly interpolates between values to find matches. The result of this rendering technique is visible in Figure 10. The method also uses a modified ray marching technique.

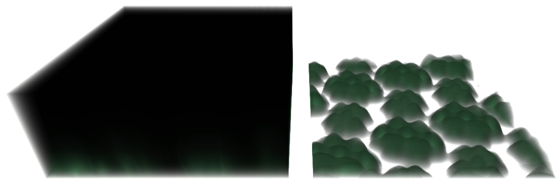

Figure 9: Volume data rendered without (left) and with (right) threshold value (5.282411e-10). With transfer function Olive for RGB and alpha value 0.1. The used dataset is PTCDA on Ag(111).

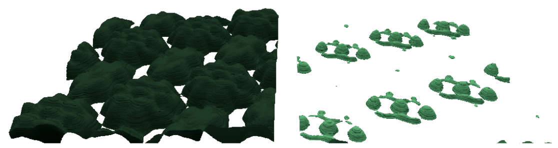

Figure 10: Exact value (5.282411e-10, 1.648464e-09) visualization of a volume dataset. With transfer function Olive for RGB. The used dataset is PTCDA on Ag(111).

Another ray marching variant is the convex visualisation, where the user can place up to six planes in the VE to cut off insignificant parts of the rendered volume. The method is described in Figure 11. This visualization offers the possibility to analyze a certain part of the volume data.

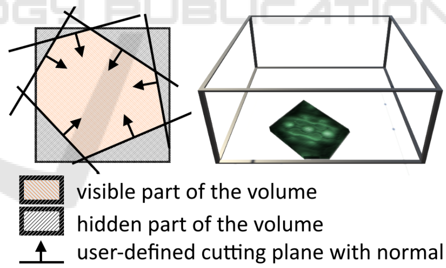

Figure 11: Convex visualization.

The slice visualization described in Figure 12 is also a valuable visualization variant. The user can move one or more planes within the VE to visualize only the overlapping part of the volume. This visualization doesn't use ray marching and is therefore significantly more performant than the other variants and thus also suitable for weaker hardware.

All these visualizations are real-time capable and also work in VR.

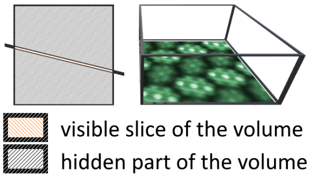

Figure 12: Slice visualization.

4.3 Transfer Function

The transfer functions are seperated for RGB and alpha. Due to the popularity of the Gwyddion software among SPM scientists, we decided to support the Gwyddion format for the RGB transfer functions as well. Thus user can use their usual transfer functions, which simplifies the analysis of the data. Any grayscale image can be used for the alpha transfer function.

5 HAPTIC FEEDBACK

The application supports four unique feedback models: collision, force, vibration and viscosity.

While the *collision model* prevents the stylus probe e. g. from a Touch X device from penetrating a measured surface by a rapid counter force, the *force model* will instead apply a smoothly in- or decreasing force in correspondence to the distance to a certain point on the surface. This in- and decreasing intensity field is also used to control the *vibration feedback*. *The viscosity* model emulates a resistance force that is related to a physical fluid with a certain viscosity. The different models are further descripted in depth in the following sections.

5.1 Haptic Device

To achieve the different feedback models, the software uses the Haptics Direct plugin from 3D Systems for Unity. It supports the 3D Systems Touch (formerly Geomagic Touch / Phantom Omni), the 3D Systems Touch X (formerly Geomagic Touch X / Phantom Desktop), and Phantom Premium models. Our test setup uses the Touch X, but the other mentioned hardware should also be supported.

The device has a maximum exertable force of 7.9 N and a continuous exertable force of over 1.75 N. It should be mentioned that although the device can apply a force of 7.9 N, this is only for a fairly short time. In practical tests, the 1.75 N therefore proved to be more reliable and sufficient for a long-lasting force. In addition, the workspace is not large enough (160 x 120 x 120 mm) to accurately examine a data set at high resolution (3D Systems, 2022). To solve this problem, additional input devices (joystick, motion controller) are used to change the position and scale of the dataset in the virtual environment. The Touch X is based on a device developed by Massie and Salisbury in 1994 (Massie and Salisbury, 1994).

To determine the position of the haptic device at runtime within the VE, it is necessary to connect the Touch X to a compatible tracker. These are available from different manufacturers, in our case it is an HTC VIVE Tracker (3.0), Figure 13.

Figure 13: Left: The 3D Systems Touch X with an HTC VIVE Tracker (3.0). Right: The virtual device tracked in the VE.

5.2 Collision

The collision feedback can only be applied to image data and should only be used in conjunction with terrain visualization. The functioning of the collision feedback can be seen in Figure 14. The haptic device tries within its capabilities to prevent the virtual device from penetrating the dataset.

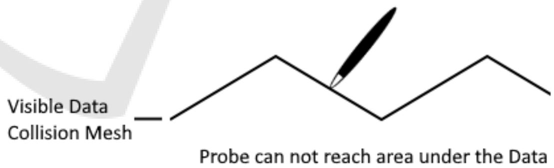

Figure 14: Collision feedback for image datasets.

The collisions are generated by the Haptics Direct plugin and Unity's physics engine. Contact points are generated based on the collision mesh and the plugin evaluates the reachable area based on them. The applied force is in tangent space in surface normal direction.

5.3 Force and Vibration

The force and vibration models can be used with image and volumetric data. For the image data, the intensity of the force and vibration feedback is calculated based on the distance from the displayed surface. The principle is illustrated in Figure 15. The further the virtual device is below the dataset, the stronger the feedback becomes. After a certain point, the limitations of the device make it impossible to increase the intensity any further. The force is always directed upwards.

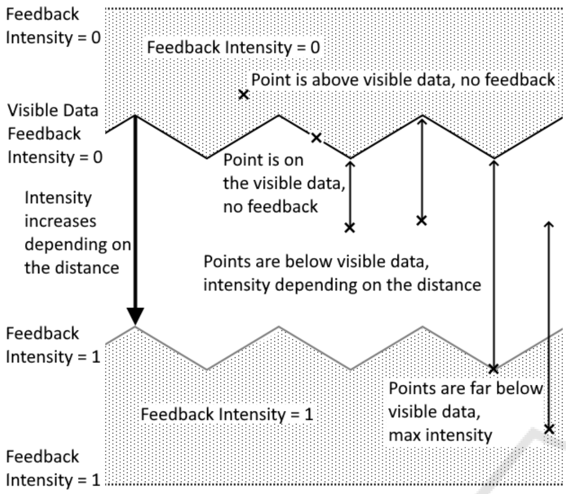

Figure 15: The determination of feedback intensity by force and vibration for image datasets.

For the volume datasets, the intensity for the force and vibration feedback is calculated via the deviation of the value at the sensing position from the target value. Several transfer functions have been developed for the determination of the intensity. The First Approach increases the intensity when the current value is lower than the intended value. Another transfer function increases the intensity at higher deviation from the target value. The last approach increases the intensity at lower deviation from the searched value. The direction of the force is always upwards. For the second variant, this pushes the haptic device to the threshold value. In the third variant, the haptic device is pushed away from the desired value.

5.4 Viscosity

Viscosity feedback is only available for volumes. The effect is achieved by setting a force that acts against the user in any direction. The applied force is calculated with a transfer function and the value at the particular position inside the volume. Formula 1 displays the calculation of the force.

$$\vec{F} = c(-\vec{v})x \qquad (1)$$

The value $c \in [0,1]$ can be set by the user at runtime to adjust the maximum force and $\vec{v}$ is calculated by the Haptics Direct plugin based on previous movements. The last step is to multiply with $x \in [0,1]$, that is the normalized sampled value at the actual probe position, thus creating a stronger counterforce at higher values.

5.5 Python Interface

In addition to the already available haptic models it is possible for the researchers to create new effects at runtime. For this reason, a Python interface for the application was developed. The application includes IronPython, which supports Python 3.4 and includes libraries and default Python scripts to calculate the intensity. It is also possible to install additional libraries, with some restrictions. The Python interface is shown in Figure 16. The input and output of the interface are predefined and given by the application.

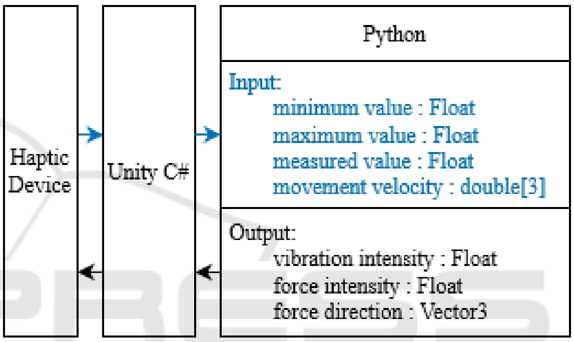

Figure 16: Overview of the Python interface.

In addition to the actual value, the minimum and maximum values are also provided to the researchers. These are necessary, for example, to interpolate the value within the limits. The velocity can be used to create interesting effects like the viscosity.

Such a haptic model can be easily created by the researcher in order to meet certain requirements, that were not yet foreseeable during development of the application. All changes to the Python script are applied directly to the runtime environment without the need to rebuild the application nor further programming knowledge.

Another benefit of the Python interface are changeable transfer functions, which are used by the haptic models to determine the intensity of the feedback. Instead of creating new haptic models the researcher can change and manipulate the used transfer function for the predefined haptic models (force, vibration and viscosity) at runtime with the same Python interface.

6 INTERACTION

The user can manipulate the datasets at runtime in VR. The application supports motion controller to move, rotate and scale the virtual representation of the dataset in VR in an intuitive way as shown in Figure 17. Translation and rotation can be achieved by one hand grabbing the dataset, then the user can move or rotate the dataset, afterwards the dataset can be released to stop the manipulation. Scaling requires two motion controller. The researcher must grip the dataset with both hands. Then it is possible to move the hands towards or away from each other to scale the dataset down or up.

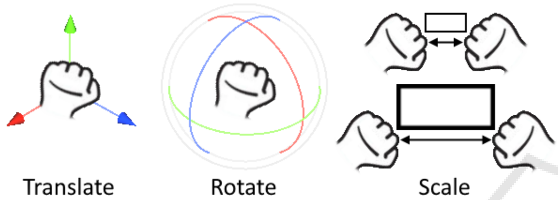

Figure 17: Hand interactions.

It is also possible to manipulate the dataset with a hall effect 3DoF joystick. This type of interaction is less intuitive, but could be more precise than the direct interaction with "floating" motion controllers. Buttons are used to switch between translate, rotate and scale modes, after which the virtual dataset can be changed separately on the axes using the joystick.

One clear advantage of the joystick interaction is that it can also be used without VR. This means that researchers do not have to learn different operating concepts for VR and for running the application on an ordinary monitor.

Another way of interaction is to change the render parameters at runtime. As mentioned in the previous sections, the data is normalized during visualization, as default values the application uses the minimum and maximum value of the dataset for normalization. These can also be adjusted at runtime to use the full resolution of the RGBA transfer functions for a subset of the data. Other values that can be changed by the researcher at runtime are the threshold value and the searched value for the exact value visualization.

7 CONCLUSION

While the application is still work in progress, we already observed positive impacts on interacting with SPM datasets. The application allows image and volume datasets to be analyzed haptically and stereoscopically and has added value compared to a purely 2D visual examination. As common in SPM data analysis.

The feedback for the visualizations was positive. In the case of 2D datasets, the visualization as terrain has been particularly well received. For the 3D datasets the result is not so clear, in the tests so far each visualization was popular and it seems like it depends more on the specific dataset which visualization is more suitable.

The haptic feedback was found to be helpful. For image data, the force model was the most convincing, because this seems to be most realistic for the users. The vibration was also perceived as positive, but was less popular. The collision model was found to be interesting, but was less relevant for practical tasks. However, this model becomes increasingly interesting when considering the context of teaching, where students can actually sense the nanostructured surfaces. This could lead to better and more sustainable nanoscience education.

The feedback for the volume data was also positive. However, there is no clear favorite here. What was surprising here was that vibration was also rated as useful for certain applications. This is particularly interesting since this can already be implemented with inexpensive devices. For the calculation of the intensity, the approach with increasing intensity at higher deviation is more popular than the other approaches.

Despite the positive feedback, there are still ideas for improvements. An enhancement would be a minimap that the user can use to navigate themselves within the data. In addition, it is planned to be able to control the SPM directly and remotely in the future. Further potential for improvement exists in the creation of digital twins for the HIDs. While the Touch X is already visually represented in the virtual environment, this feature is missing on other HIDs, that a researcher might use. To solve this problem, we are currently experimenting with visualizing the real workplace as a point cloud in the virtual environment. Another approach is the spatial registration of the HIDs through optical tracking techniques. Regardless of the potential for improvement, the application has already proven useful in initial practical tests.

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