# A Simultaneous 2D/3D Autostereo Workstation

Dennis Chau<sup>*a*</sup>, Bradley McGinnis<sup>*a*</sup>, Jonas Talandis<sup>*a*</sup>, Jason Leigh<sup>*a*</sup>, Tom Peterka<sup>*b*</sup>, Aaron Knoll<sup>*b*</sup>, Aslihan Sumer<sup>*b*</sup>, Michael Papka<sup>*b*</sup>, and Julius Jellinek<sup>*b*</sup>

<sup>*a*</sup>Electronic Visualization Laboratory, University of Illinois at Chicago <sup>*b*</sup>Argonne National Laboratory

# ABSTRACT

We present a novel immersive workstation environment that scientists can use for 3D data exploration and as their everyday 2D computer monitor. Our implementation is based on an autostereoscopic dynamic parallax barrier 2D/3D display, interactive input devices, and a software infrastructure that allows client/server software modules to couple the workstation to scientists' visualization applications. This paper describes the hardware construction and calibration, software components, and a demonstration of our system in nanoscale materials science exploration.

**Keywords:** Information interfaces and presentation; Multimedia information systems; Artificial, augmented, and virtual realities.

# **1. INTRODUCTION**

Scientific data, fueled by growth in computing power and physical sensor resolution, offer the possibility to explore phenomena from the scale of the universe to subatomic particles. While our ability to simulate and collect scientific data is unprecedented, it brings with it new challenges for interactive exploration. Along with increased data size, datasets are increasing in complexity, with many quantities represented over complex field geometries. These geometries are frequently 3D spatial or 4D spatio-temporal, and 2D visualizations alone cannot capture the information contained in high-dimensional data.

This paper presents our development of an immersive desktop autostereoscopic workstation, driven by the needs of nanoscale materials science for the exploration of structures used in energy research. One example of energy research being conducted at Argonne National Laboratory is the design of amorphous carbon structures for new anode materials in next-generation batteries. These structures, consisting of diamond cores surrounded by sheaths of graphite, provide increased area for trapping lithium ions in electrolytes. Figure 1 shows that complex models consisting of 700,000 atoms are difficult to view and understand using traditional display techniques that flatten deep structures onto a single view plane. Motivated by this example and others encountered in the United States Department of Energy's Energy Frontier Research Centers, we propose a new work environment for scientists.

Send correspondence to dchau1@uic.edu



Figure 1. Ball-and-stick rendering without and with volume visualization. Stereo display is indispensable for visualizing such large and complex structures.

One of our objectives was to deploy a transparent environment that directs the user's focus on the science problem instead of the technology. Toward this end, we employed innovative autostereoscopic hardware and software that affords novel user interactions. Another goal was to support existing workflows so that scientists need not give up tools upon which they rely to be productive. We coupled our workstation to remote visualization applications to satisfy this goal, instead of developing a new system for producing virtual imagery. Lastly, we wanted an accessible environment is always available and requires little or no added effort on the part of the user. Today's science work day is fluid and consists of many interleaved tasks, so having to plan and reserve "3D time" to use high-end resources such as CAVEs can cause such facilities to be underutilized. Instead, we bring the immersive environment to the scientist's desktop, where it is always on, requires minimal gear to use, and supports 3D data exploration at the same time as 2D tasks such as email and document writing.

This paper summarizes our implementation of the next generation of the Dynallax dynamic parallax barrier autostereoscopy system in a desktop form factor and a demonstration of its use in materials science. It is driven by a software system called DVC, or dynamic view client, that couples existing visualization applications to the hardware. DVC consists of two parts: a server-side library that enables streaming of stereo image pairs to the client side and interacts with applications to process client input; and a client-side library that displays stereo images, supports interaction devices, and combines 2D and 3D work spaces.

## 2. BACKGROUND

A review of earlier stereo and autostereo virtual environments shows that usability for science can be an elusive goal. Anaglyph stereo discards much of the color spectrum and hence is not useful for scientific visualization. Field-sequential and passive polarized stereo require glasses, which inhibit multitasking between 2D and 3D tools. Lenticular automulti-scopic displays compress depth and are not first-person head-tracked. Varrier<sup>1</sup> static parallax barrier displays cannot switch between 2D and 3D mode because of the presence of a fixed parallax barrier.

In their paper Lee et al.<sup>2</sup> discuss the development of the field of autostereo and how it must accommodate 2D content. With the majority of content currently available being 2D, it is easy to see why this is so. The authors explain how current parallax barrier devices use a time-multiplexed barrier to achieve a "2D only" mode. However, our device goes beyond having a separate 2D and 3D modality and offers a mixed 2D/3D paradigm, allowing users to view both types of content simultaneously. Steinicke et al.<sup>3</sup> research this concept of mixed 2D/3D content on autostereo displays and refer to it as interscopic. In their research they outline a method for mixing the 2D user interface for CAD software with a stereo rendering of the model being designed. In their research, an informal survey showed that interscopic user interface design may benefit certain technical applications.

There are a number of other parallax barrier devices being developed commercially as well as in academia. One such device was Varrier,<sup>4</sup> that used a static barrier printed on glass. There is also the device produced by Lanman et al.<sup>5</sup> which has two LCDs layered, with one acting as a dynamic barrier. This is a very similar design to our own except the Dynallax alters the barrier based on head position, where as Lanman's device alters the barrier based on the content of the scene being rendered. This solves some of the issues that are present in our system but it also introduces some new issues such as flickering. Finally, Stolle et al.<sup>6</sup> introduce an autostereo device being developed in industry. Although it does not utilize a parallax barrier, it has many common goals with the Dynallax workstation including autostereo, simultaneous 2D/3D, and compatibility with existing OpenGL applications. Its main target audience is "hardcore" game players.

There have been many advances in immersive stereoscopic systems and technology over the last two decades. One application area that has the potential to take advantage of these advances is domain science. For example, in their project GROPE, Brooks et al.<sup>7</sup> provided visualizations of molecules and their force fields to chemists trying to discern docking patterns of drugs. The authors report that because of the immersive interactions with the GROPE system, chemists had a new understanding of drug docking and receptor site interactions, increasing their situational awareness.

Another project, called Crumbs, was developed by Brady et al.<sup>8</sup> at the University of Illinois Urbana-Champaign for use in a CAVE<sup>9</sup> system. Crumbs visualized volumetric data and provided easy and intuitive ways for users to navigate and inspect the datasets. When used by biologists from various domains, they reported that Crumbs improved workflow and contributed to increased understanding of the data, acknowledging its educational possibilities.

As a final science application, Bohrer et al.<sup>10</sup> showed that a group of interdisciplinary scientists could collaborate in an immersive stereo environment, in this case the Duke Immersive Virtual Environment. Using a visualization, these

scientists were able to explore a large complex dataset whose variables interacted in a nonlinear way. Their access to this immersive stereo environment proved to be fundamental to synthesising a hypothesis about the dataset. Unlike these large-scale specialty displays, we attempt to bring the advantages of these immersive stereoscopic displays to the scientist where they work, and to accommodate daily activities in addition to providing novel data exploration.



The work presented here is a continuation of the Dynallax system<sup>11, 12</sup> development and the software that drives it, Dynamic View Client (DVC).<sup>13</sup> DVC leverages OpenGL shaders and MPI<sup>14</sup> to maintain a dynamic parallax barrier and a corresponding interlaced stereo image. Previously, developing Dynallax applications often required altering the DVC library itself to manage custom input events and new input devices. DVC also did not include a mechanism for modifying coupled visualization applications, nor did it afford 2D/3D simultaneous workflows. The new work presented in this paper streamlines the application development process on both the client and server sides by abstracting more of these details.

#### 3. METHOD

Dynallax incorporates a hardware and software infrastructure in order to create a hybrid 2D/3D scientific workstation. The hardware infrastructure is described by the specifications and parameters for our dynamic parallax barrier display. The software infrastructure provides a transparent environment for both developers and scientists, achieved by abstracting stereoscopic rendering, input from novel user interfaces, and 2D/3D windowing.

## 3.1 Hardware

Our display assembly can be seen in Figure 2 and uses the Dynallax method to create 3D images by means of a dynamic parallax barrier.<sup>11</sup> This method leverages the stacking of two LCD panels, one in front of the other. The interleaved scene image is drawn on the rear screen, with the dynamic parallax barrier generated on the front screen. Altering this dynamic parallax barrier programmatically provides the 2D/3D windowing capabilities not found in static parallax barrier devices such as Varrier.<sup>4</sup>

The rear 'data' screen, is a stock Apple Cinema 30 inch LCD display. This display was chosen for its high (2560 x1600 pixel) resolution, brightness (400 cd/m<sup>2</sup>) and professional image quality. The front 'barrier' screen is the LCD panel extracted from a Dell 3007WFP-HC display of the same size and resolution. The Dell's power and display components are retained in order to operate and drive the LCD panel. Its enclosure, backlight and interface electronics are not required and removed. The LCD panels are stacked face-to-face to align their interior polarization layers and allow light to pass through both panels and eliminate the need to remove any polarization layers from the bonded panel assemblies. The two LCD panels are visually aligned by pixel row using simple line patterns drawn on each LCD prior to mechanical fixing.



Figure 3. User multitouch interaction

The combined display assembly is mounted to an extruded aluminum framing enclosure providing for +/- 20 degree view angle adjustment. To assist in scientific discovery, lightweight user interaction devices are included. Touch capability is provided by a PQ Labs Multi-Touch 32" G3Plus touch screen, an infrared-based overlay framing the display surface and providing up to 32 simultaneous touches and/or gestures for application control and interaction with images. Additionally, head tracking is provided by a TrackIR v.5 tracking system, requiring users only to wear a lightweight visor and providing nonintrusive head tracking capability. A Wiimote 3D controller is also provided. User interaction is shown in Figure 3.

Figure 2. The Dynallax display system

Dynallax is powered by an Ubuntu Linux workstation with dual Intel Xeon 2.4GHz processors, two NVIDIA GTX 460 (1 GB) GPUs, and 12 GB RAM.

#### 3.1.1 System Configuration

The front and rear screens are each connected to a different graphics card, but the screens are combined side-by-side into a single canvas using Xinerama mode, so that the front screen is to the right of the rear screen in the configuration.

USB drivers for the TrackIR camera and the PQLabs touch screen are not available for Linux, so we installed a virtual machine (VM) running a Windows-7 64-bit enterprise edition guest operating system (OS) on top of the Linux host OS. We selected the free VMware player over other VM software because of its support for USB devices. We set the network to bridged mode, so that the guest and host each have their own IP address, and we allotted 2GB of memory to the guest. The remaining VM settings remained at their default values.

The Windows guest OS runs two utility programs that we wrote. A tracker server utility grabs raw head tracker coordinates and sends them over the loopback network interface to the Linux host on a specified port, and a touch server utility does the same for touch screen data. The virtual machine and utility programs only need to be started once and execute continuously in a minimized state. We have not experienced any noticeable lag due to using a virtual machine to drive the head tracker and touch screen.

## 3.1.2 Optical Parameters

The Nyquist Sampling Theorem states that each ray of light entering an eye be generated from at least two pixels, making the minimum barrier period 4 pixels wide.<sup>4</sup> A larger period means that more pixel samples contribute to each channel, contain larger guard regions, and further improve image quality. A larger barrier period, however, results in barrier lines that are more visible, so there is a trade off between crosstalk and barrier visibility. In our experiments, we empirically found that an ideal compromise for Dynallax is a barrier period of 6 pixels (0.060 in., or 1.5 mm). Table 1, a complete list of optical parameters, shows that we are slightly below that target in our construction, approximately 5.25 pixels.

From the target barrier period, the physical separation between screens is computed as follows. From Peterka et al.,<sup>12</sup> optical thickness *t* is a function of the optimal viewing distance  $z_{opt}$ , interocular distance *e*, and barrier period *p*, and  $t \approx z_{opt} p/2e$ . For a desktop display, we use  $z_{opt} = 24$ in. (609 mm), resulting in an optical thickness of t = 0.288in. (7.3 mm) To find the physical separation between the two LCD panels, we subtract the thickness of one LCD glass, divided by its refractive index, resulting in a 0.236 in. (5.99 mm) air space between the LCDs. We then selected spacer materials that were readily available in stock thicknesses, which resulted in the parameters in Table 1.

## 3.2 Software : Dynamic View Client (DVC)

The overall system architecture is shown in Figure 4. Dynallax's Dynamic View Client (DVC) software consists of

Table 1. Major Optical Parameters				
Parameter	Value			
Screen Size	25.6 in x 16.0 in (650 mm x			
	406 mm)			
Screen Base Resolution	2560 x 1600			
Effective Resolution	640 x 1600 per eye			
LCD Pixel Pitch	0.010 in (0.25 mm)			
Barrier Period	0.052 in (1.32 mm)			
Barrier Duty Cycle	0.75 black, 0.25 white			
Screen Separation	0.212 in (5.38 mm) air + 0.078			
	in (1.98 mm) glass			
Optical Thickness	0.264 in (6.71 mm)			
Optimal View Distance	24 in (609 mm)			
Interocular Distance	2.5 in (63.50 mm)			

two parts: DVCLib and DVCSdk. DVCLib is linked to a rendering application running on our workstation, and DVCSdk is linked to a visualization application that could be running on the same or a remote machine. DVCLib and DVCSdk work together to couple local rendering with remote visualizations as follows. DVCSdk sends stereo image pairs from the remote visualization to DVCLIb, which renders autostereoscopic imagery, manages simultaneous 2D/3D windows, catches user input events, and sends them to DVCSdk. DVCSdk receives user inputs and makes them available to the visualization application so that it can update its state accordingly. The three main abstractions used to achieve this coupling: stereoscopic rendering, input device handling, and 2D/3D window management, are described in further detail below.



Figure 4. The overall architecture of DVC shows how the three major abstractions couple local and remote rendering, capture user input, and integrate 2D and 3D windows. The visualization application can run either on the same physical machine or remotely.

## 3.2.1 Stereoscopic Rendering Abstraction

Parts of stereoscopic rendering occur in both the remote visualization application as well as in the local rendering application. The visualization application performs the initial rendering of stereo image pairs and transmits them to the rendering application for final autostereoscopic interleaving and rendering on the Dynallax device. The rendering and image communication protocol are described below.

The visualization renders scientific data. This application can be an existing piece of software such as Paraview,<sup>15</sup> or it can be a custom application to suite the needs of domain scientists such as our materials science visualization tool, Nanovol.<sup>16</sup> In either case, it is responsible for taking user input events and head tracker data and using these inputs to modify the scene. The result is a stereo pair of left- and right-eye views of the dataset. With the help of DVCSdk, these stereo pairs are sent to the rendering application.

The rendering application processes the stereoscopic pairs for display on the Dynallax front and rear LCDs. The process involves interleaving the left and right images and rendering the result on the rear LCD, while computing and rendering the parallax barrier on the front LCD. The calculations for both the parallax barrier and the autostereo scene interleaving are adopted from the Dynallax rendering algorithm.<sup>11</sup> To achieve accurate autostereoscopy, the front and rear LCDs need to be synchronized properly. The synchronization and rendering are handled via MPI and managed by DVCLib, so that simply linking DVCLib into the rendering application abstracts these functions from the user.

The transfer of the stereo image pairs between DVCLib and DVCSdk is done using TCP sockets. The TCP networking protocol was chosen to ensure that image data was not lost or reordered. The protocol in Peterka et al.<sup>13</sup> sends each image as packets consisting of a header followed by image data. The 12-byte header is used to determine the size of the image and whether it is a left or right image of the pair. The image is 3 bytes per pixel, RGB format. This remote rendering protocol allows the visualization application to dynamically modify the autostereo image size. The stereo pairs rendered by the visualization application do not have to match the resolution of the rendering application; DVC automatically handles scaling between the visualization application window size and and the rendering application window size.

#### 3.2.2 Input Device Abstraction

Local user input events are collected by DVCLib within the rendering application. Meanwhile, DVCSdk, at the visualization application, accesses the interaction data via streams that are managed by a library called OmegaLib.<sup>17</sup> The OmegaLib infrastructure handles a majority of the message passing and event queueing as follows. Omegalib is a middleware designed to ease the development of applications on virtual reality and immersive systems by encapsulating a wide range of input peripherals: controllers, motion capture systems, touch surfaces, and so forth. Its abstraction helps users connect to various devices and grab input data. The input data are processed and repackaged as a generic event packet that consists of an event type and related data. Two examples of event types include rotations and screen touches, with corresponding data consisting of degree of rotation and touch position. OmegaLib also supports the generation of custom event packets. Once generated, the event packets are stored in an *EventList*.

Additionally, OmegaLib has server/client capabilities, as it was developed to be an effective method of transferring abstracted user input from a local system to a remote system. The OmegaLib server, *OInputService*, abstracts input into event packets and stores them in an EventList. The event packets can be streamed to any connected external application. The external application can also include the OmegaLib client, *OInputClient*. This allows the application to receive the abstracted events and place them in a separate event list for easy access.

DVCLib wraps both an OInputClient and an OInputService in a *DVCDataHub*. The DVCDataHub acts as a client by receiving event data from the Windows virtual machine. The virtual machine executes OInputService to gather input data from devices such as the touch screen and the head tracker, and additional abstraction functions were also written to generate custom event packets for the 3D remote controller, mouse, and keyboard. Once collected and processed, the events are streamed to the DVCDataHub and collected in the EventList. In the visualization application, DVCSdk uses a thread to continuously poll and stream events from DVCLib's data hub. This provides user interaction data from novel devices to the visualization application so that it can alter the scene and render new stereo pairs.

#### 3.2.3 2D/3D Window Abstraction

Dynallax can be used simultaneously as a 3D lens into scientific data and as a 2D workstation for everyday tasks such as word processing or web browsing. It does so by maintaining information about 2D windows on the rear screen that would be occluded by the parallax barrier on the front screen. Dynallax uses this information to clear regions of the front screen when these rear screen windows are brought into focus. This functionality is delivered in a custom X11 window manager that we implemented within DVCLib. This way, all original 2D software can run unimpeded at native resolution, and 2D and 3D windows can be resized, moved, and switched in and out of focus seamlessly. For example, Figure 5 shows a 2D web browser running alongside the 3D autostereo Nanovol application.

X11 is the primary window system in the Dynallax workstation, and XLib is the C library used to interface with the window system. X11 uses a tree structure to maintain information about the various windows on the screen. By polling the root or main window at every frame, a list of all the windows on the screen



Figure 5. Example of 2D web browsing simultaneous with 3D molecular modeling.

can be determined. The properties of each window are stored in the XWindowProperties data structure. From this structure, knowledge of the window's name, size, location, and Z depth can be determined. This knowledge is used to determine if a window needs to be cleared and if so, the size and location of the clearing area. Additionally, the location can be used to identify windows that are on the front LCD. Since the front LCD is mounted upside down, XLib is also used to prevent 2D windows from being moved to the front screen where they would appear inverted. Such windows, identified by their window coordinates, are automatically shifted to the rear screen.

At every frame, each window is checked to see whether it interacts with the parallax barrier. A window's name attribute is used to distinguish between 2D windows and our autostereoscopic 3D windows. The Z depths of 2D windows are compared to our 3D parallax barrier window, and for 2D windows on top of our 3D window (in terms of their focus or Z depth), the parallax barrier needs to be cleared based on the size and location of the 2D window. Windows to be cleared are rectangular, and their context is stored in an array. This array is used when DVCLIb renders the parallax barrier via GLSL shaders, as the array is passed into the GPU. There, after the parallax barrier has been rendered in the frame buffer, a white rectangle is drawn for each window context. The resulting white region is the union of all the 2D windows that are on top of the parallax barrier window, in terms of the their Z depth. The transparent nature of the front LCD allows the user to see through the white region to the 2D windows on the rear LCD.

# 4. RESULTS AND CASE STUDIES

We evaluated our workstation by measuring optical parameters such as crosstalk and scattering. We then coupled Dynallax to three materials science applications that visualized isosurfaces, ball-and-stick models, and volume rendering. We also measured end-to-end frame rates for several configurations of these applications.

## 4.1 Optical Tests

We evaluated the optical quality of the system using a variety of methods. The contrast ratio was measured as the difference between light emitting from both screens set to full white compared to both screens set to black, a ratio of 64:1. A test of light leakage from a white rear screen through a black front screen resulted in 2% leakage, or 98% opacity of a black front screen. We tested crosstalk using two methods; both resulted in a crosstalk ratio of 25%. The first method from Sandin et al.<sup>4</sup> measures the light levels in one eye channel set to black and one eye channel set to white, and computes the ratio of the black to the white intensity.



Figure 6. Photographic measurement of crosstalk. Primary channel is a brighter cube at the left and the crosstalk to its right shows a faint ghost image.

The second method relies on digital photographs of the primary and crosstalk channels for a single eye position. By photographing the same image at different shutter speeds and comparing the results, we can find the faster shutter speed that reduces the primary channel to the same intensity as the crosstalk at the original shutter speed. The ratio of these speeds is the crosstalk per eye. We conducted this experiment with the camera fitted with an 8 mm entrance pupil, to mimic the human eye, and the result is shown in Figure 6. The bright cube in the left half of this image is the primary channel, and the dim ghost on the right side is the crosstalk. The same shot taken at a four times faster exposure resulted in approximately the same intensity primary channel as the crosstalk in the original image of Figure 6.



Figure 7. Comparison of text displayed in 2D on a comparable single-layer LCD monitor (left) and similar text displayed in 2D on our Dynallax system (right) reveals significant light dispersion due to internal reflections.

This was a surprising finding compared to the 10% crosstalk reported in 2007.<sup>11</sup> We postulate that our current implementation, which is constructed from off-the-shelf components, has different optical characteristics than the implementation used previously, which was based on a product commercially designed to function as a 2-layer display. Specifically, we studied light scattering caused by what we think are internal reflections in our current design.

Figure 7 demonstrates of the problem by showing plain text displayed on two monitors. A single-layer LCD display of the same model as our Dynallax rear screen is shown at left, compared to text displayed on our Dynallax display in 2D mode at

right. The glow around the characters in the right image indicates significant light scattering.

To measure the percentage of scattering, we displayed a checkerboard pattern on the Dynallax display in 2D mode. Each square is  $5 \times 5$  pixels, the same size as one barrier period. Light scattering appears as a gray gradient bleeding into the black squares of the photographed pattern. The original photograph is shown in the left image of Figure 8. The center image shows a Gaussian blur of radius 3 applied to the image to filter out high-frequency noise. As in the crosstalk test, we photographed a series of images at shorter exposures until the lighter squares in the dark-ened images matched the intensity level of the dark squares in the original image. This image is at the right of Figure 8 and corresponds to a



Figure 8. The amount of light scattering can be measured by displaying a checkerboard pattern in 2D mode in Dynallax and photographing at different shutter speeds. Left: original photograph shows light leaking from the white regions in a gray gradient. Center: same, with 3-pixel Gaussian low-pass filter. Right: same, taken at 13% shorter exposure.

scattering ratio of 13%, a significant contributor to the crosstalk that we observed.

# 4.2 Use Cases

We employed our autostereo environment in three applications visualizing molecular models in materials research. This field in particular benefits from stereo vision, as it frequently involves ball-and-stick models that suffer from occlusion as the number of atoms increases. To accomplish this, we coupled DVC with Nanovol, an interactive visualization tool designed for mixed ball-and-stick and volume rendering for these materials applications.<sup>16</sup> Since many materials volume datasets are low-resolution, Nanovol employs tricubic B-spline filtering to improve visual quality and reconstruction of sharp features. However, our autostereo framework would extend to any application that can output stereo images and receive appropriate inputs.



Figure 9. Comparative visualization of amorphous aluminum nanobowls demonstrates arranging and viewing models in 3D space according to different model parameters.

The first materials application involves comparison of amorphous aluminum oxide nanobowls, which serve as catalyst support structures. A molecular dynamics system simulates atomic diffusion at various temperatures. Depending on the radius of the bowl and temperature of the system, the compound may lose its structure. Domain scientists wish to examine the output of multiple simulations, and compare which parameters lead to stable or unstable bowl structures. We model this geometry as solventaccessible molecular surfaces using SURF,<sup>18</sup> and use DVC to visualize the resulting triangle meshes. Conventionally, depth in these models is indicated by a RGB colormap, which can be difficult to perceive in anaglyph stereo systems. Autostereo displays allow for 3D depth perception without sacrificing color range (Figure 9).

Larger ball-and-stick models benefit strongly from stereo display. Ball-and-stick is the conventional rendering modality for most chemistry applications. However, it is often impractical to render even moderate-size models (1,000 atoms or more) in this fashion. In current materials research it is common to work with models with thousands to millions of atoms. While fog and volume rendering improve depth intuition, they obscure objects in the background. Figure 1 shows a portion of a 740,000 atom carbon nanosphere structure, with and without volume rendering, and displayed with our autostereo system.

Another use case for stereo rendering is modeling initial atom geometry prior to optimization in density functional theory (DFT) computation, for example in NWChem.<sup>19</sup> Domain experts spend significant time manipulating models in molecular modeling software such as Avogadro.<sup>20</sup> The goal is to place atoms of interest sufficiently close together that one can simulate formation of chemical bonds. Though modeling software provides some automatic optimization functionality, in practice many molecules are initially modeled by hand. Unoptimized geometry can result in nonconvergent DFT computation and wasted computation time. Due to the added depth cues, stereo display can aid in modeling initial geometry. After the DFT computation is performed, we can visualize the resulting optimized atom geometry and the electron density field, a volume dataset. An example illustration, modeling CO adsorption on a platinum catalyst cluster, is shown in Figure 10.

### 4.3 End-to-End Performance

Frame rate performance of various use cases, at various frame buffer sizes, is shown in Table 2. In all examples, we ran Dynallax at 2500x1600 resolution, on an NVIDIA GTX 480 GPU. In the top two cases, we ran DVC in a standalone mode rendering a previously generated mesh, while in the bottom nine cases, we run Nanovol as a coupled application on a separate NVIDIA GTX 480 in the same workstation, producing images at varying



Figure 10. CO adsorption on a platinum cluster, an example of DFT computation on manually modeled molecular geometry.

resolutions. When rendering mesh geometry directly in Dynallax, as in the first two cases, performance is limited by the aggregate amount of geometry. For coupled applications, performance is limited by the visualization application and the communication delay between the two applications. For coupled applications, we find performance is consistently interactive at small frame buffers (660x400), and between 2-15 fps for larger buffers (1320x800). These tests were conducted

Data	Geometry	Data Size	Framebuffer	Coupled	FPS	
nanobowl	molecular surface	196k triangles	2500x1600	no	50	
nanobowl x12	SAS triangle mesh	2390k triangles	2500x1600	no	10	
nanosphere	stick	92k atoms	1320x800	yes	8.0	
nanosphere	volume	490x512x512 volume	1320x800	yes	5.2	
nanosphere	stick+volume	>> >>	1320x800	yes	2.6	
nanosphere	stick+volume	,, ,,	660x400	yes	5.3	
CO-Pt7 DFT	volume	9 atoms, 101x101x101 volume	1320x800	yes	6.0	
CO-Pt7 DFT	ball+stick+volume	>> >>	1320x800	yes	9.6	
CO-Pt7 DFT	ball+stick+volume	,, ,,	1320x800	yes	4.5	
CO-Pt7 DFT	ball+stick+volume	,, ,,	660x400	yes	12.9	
CO-Pt7 DFT	ball+stick+volume	,, ,,	400x300	yes	28.0	

Table 2. Performance for Various Use Cases

using synchronous coupling, and we expect that our next asynchronous version will allow DVClib at the rendering side to run at 60 fps independent of the frame rate of DVCSdk at the visualization side.

#### 5. SUMMARY

We presented an autostereoscopic hardware and software solution that is designed to transparently support scientists' daily work. Without the need for a lab or dedicated space, Dynallax is one display system for both data exploration and office tasks, and it supports a variety of input devices. Dynallax enables scientists to couple existing and new visualization applications to it with minimal modification. We demonstrated its use in the exploration of materials science models.

We implemented several hardware features, including high-resolution dynamic barrier autostereoscopy in a desktop form factor, and a variety of interaction devices that include keyboard, mouse, 3D remote controller, head tracker, and touch screen. New software contributions include a server-side library (DVCSdk) that enables streaming of stereo image pairs to the client side, receipt of client control data, and interaction with the application to process client input. A client-side library (DVCLib) communicates with the remote visualization application, displays stereo images using autostereoscopic dynamic barrier technology, supports interaction devices, and seamlessly integrates 2D and 3D work regions in the same display.

Our evaluation did uncover some limitations of the system. The optical quality needs further improvement, and the tight frame-rate coupling to the visualization application needs to be relaxed. The set-up and calibration of a new installation also needs to be simplified. Our plans for future work address some of these limitations. The optical path will be studied in greater detail, including a brighter backlight, removal of one redundant polarizer, and mitigation of internal reflections in the optical path. We are continuing to work to decouple frame rates between server and client to allow smoother interaction, and we are also working to automate the camera calibration process.

## ACKNOWLEDGMENTS

This work was supported by the Office of Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy, under Contract DE-AC02-06CH11357. Work is also supported by DOE with agreement No. DE-FC02-06ER25777.

#### REFERENCES

- Peterka, T., Kooima, R., Girado, J., Ge, J., Sandin, D., and DeFanti, T., "Evolution of the varrier autostereoscopic vr display," in [*Proceedings of IS&T / SPIE Electronic Imaging 2007*], (2007).
- [2] Lee, B., Choi, H., Kim, J., Kim, Y., and Cho, S.-W., "Status and prospects of autostereoscopic 3d display technologies," in [*Lasers and Electro-Optics Society, 2007. LEOS 2007. The 20th Annual Meeting of the IEEE*], 354 –355 (oct. 2007).
- [3] Stenicke, F., Ropinski, T., Bruder, G., and Hinrichs, K., "Inerscopic user interface concepts for fish tank virtual reality systems," in [*Proceedings of IEEE Virtual Reality 2007*], (2007).

- [4] Sandin, D., Margolis, T., Ge, J., Girado, J., Peterka, T., and DeFanti, T., "The varrier autostereoscopic virtual reality display," ACM Transactions on Graphics, Proceedings of ACM 24(3), 894–903 (2005).
- [5] Lanman, D., Hirsch, M., Kim, Y., and Raskar, R., "Content-adaptive parallax barriers: optimizing dual-layer 3d displays using low-rank light field factorization," in [ACM SIGGRAPH Asia 2010 papers], SIGGRAPH ASIA '10, 163:1–163:10, ACM, New York, NY, USA (2010).
- [6] Stolle, H., Olaya, J.-C., Buschbeck, S., Sahm, H., and Schwerdtner, A., "Technical solutions for a full-resolution autostereoscopic 2d/3d display technology," *Stereoscopic Displays and Applications XIX* 6803(1), 68030Q, SPIE (2008).
- [7] Brooks, Jr., F. P., Ouh-Young, M., Batter, J. J., and Jerome Kilpatrick, P., "Project gropehaptic displays for scientific visualization," in [*Proceedings of the 17th annual conference on Computer graphics and interactive techniques*], SIGGRAPH '90, 177–185, ACM, New York, NY, USA (1990).
- [8] Brady, R., Pixton, J., Baxter, G., Moran, P., Potter, C., Carragher, B., and Belmont, A., "Crumbs: a virtual environment tracking tool for biological imaging," in [*Biomedical Visualization*, 1995. Proceedings. ], 18–25, 82 (oct-3 nov 1995).
- [9] Cruz-Neira, C., Sandin, D., DeFanti, T., Kenyon, R., and Hart, J., "The cave: Audio visual experience automatic virtual environment," *Communications of the ACM* 35(6), 64–72 (1992).
- [10] Bohrer, G., Longo, M., Zielinski, D., and Brady, R., "Vr visualisation as an interdisciplinary collaborative data exploration tool for large eddy simulations of biosphere-atmosphere interactions," in [Advances in Visual Computing], Bebis, G., Boyle, R., Parvin, B., Koracin, D., Remagnino, P., Porikli, F., Peters, J., Klosowski, J., Arns, L., Chun, Y., Rhyne, T.-M., and Monroe, L., eds., Lecture Notes in Computer Science 5358, 856–866, Springer Berlin / Heidelberg (2008).
- [11] Peterka, T., Kooima, R., Girado, J., Ge, J., Sandin, D., Johnson, A., Leigh, J., Schulze, J., and DeFanti, T., "Dynallax: Solid state dynamic barrier autostereoscopic vr display," in [*Proceedings of IEEE Virtual Reality 2007*], (2007).
- [12] Peterka, T., Kooima, R., Sandin, D., Johnson, A., Leigh, J., and DeFanti, T., "Advances in the dynallax solid-state dynamic parallax barrier autostereoscopic visualization display system," *IEEE Transactions on Visualization and Computer Graphics* 14(3), 487–499 (2008).
- [13] Peterka, T., Ross, R., Yu, H., Ma, K.-L., Kooima, R., and Girado, J., "Autostereoscopic display of large-scale scientific visualization," *Stereoscopic Displays and Applications XX* 7237(1), 723706, SPIE (2009).
- [14] Geist, A., Gropp, W., Huss-Lederman, S., Lumsdaine, A., Lusk, E., Saphir, W., and Skjellum, T., "Mpi-2: Extending the message-passing interface," in [*Proceedings of Euro-Par'96*], (1996).
- [15] Moreland, K., Avila, L., and Fisk, L. A., "Parallel unstructured volume rendering in paraview," in [*Proceedings of IS&T SPIE Visualization and Data Analysis 2007*], (2007).
- [16] Knoll, A., Peterka, T., Hereld, M., Papka, M. E., Liu, B., Chan, M., and Greeley, J., "A Volumetric Framework for Registration, Analysis and Visualization of Nanostructured Materials," in [Online Proceedings of SciDAC 2011], SciDAC (2011).
- [17] Febretti, A., Mateevitsi, V., Chau, D., Nishimoto, A., McGinnis, B., Misterka, J., Johnson, A., and Leigh, J., "The omegadesk: Towards a hybrid 2d and 3d work desk," in [Advances in Visual Computing], Bebis, G., Boyle, R., Parvin, B., Koracin, D., Wang, S., Kyungnam, K., Benes, B., Moreland, K., Borst, C., DiVerdi, S., Yi-Jen, C., and Ming, J., eds., Lecture Notes in Computer Science 6939, 13–23, Springer Berlin / Heidelberg (2011).
- [18] Varshney, A., Brooks, Jr., F. P., Richardson, D. C., Wright, W. V., and Manocha, D., "Defining, computing, and visualizing molecular interfaces," in [*IEEE Visualization '95 Proceedings*], Nielson, G. M. and Silver, D., eds., 36– 43 (1995).
- [19] Valiev, M., Bylaska, E., Govind, N., Kowalski, K., Straatsma, T., Van Dam, H., Wang, D., Nieplocha, J., Apra, E., Windus, T., et al., "Nwchem: a comprehensive and scalable open-source solution for large scale molecular simulations," *Computer Physics Communications* 181(9), 1477–1489 (2010).
- [20] Avogadro: an open-source molecular builder and visualization tool, http://avogadro.openmolecules.net/.

The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357. The U.S. Government retains for itself, and others acting on its behalf, a paid-up nonexclusive, irrevo-cable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government.