Snap2Diverse: Coordinating Information Visualizations and Virtual Environments

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ABSTRACT

The field of Information Visualization is concerned with improving how users perceive, understand, and interact with visual representations of abstract information. Immersive Virtual Environments (VEs) excel at a greater comprehension of spatial information. This project addresses the intersection of these two fields known as Information-Rich Virtual Environments (IRVEs) where perceptually realistic information, such as models and scenes, are enhanced with abstract information, such as text, numeric data, hyperlinks, or multimedia resources. IRVEs present a number of important design challenges including the management, coordination, and display of interrelated perceptual and abstract information. We describe a set of design issues for this type of integrated visualization and demonstrate a coordinated, multiple-views approach to support 2D and 3D visualization interactions such as overview, navigation, details-on-demand, and brushing-and-linking. In the CAVE, spatial information in a VE is interactively linked to embedded visualizations of related abstract information. Software architecture issues are discussed with details of our implementation applied to the domain of chemical information visualization. Lastly, we subject our system to an informal usability evaluation and identify usability issues with interaction and navigation that guides future work in these environments.

Keywords: Coordinated Multiple Views, Brushing, Virtual Environments, Information Visualization, Cheminformatics

1. INTRODUCTION & BACKGROUND

In many modern design and research applications, a significant proportion of data concerns geometrical and structural information as well as abstract or quantitative data associated with that geometry. This class of problems has been generally termed "Information-Rich Virtual Environments" (IRVEs) by Bowman et al [1,2,3]. An IRVE is a perceptually 'realistic' virtual environment that is enhanced with multiple information types embedded within its view construct. A VE is said to be *realistic* if its perceptible components represent components that would normally be perceptible in the physical world. As users navigate within the perceptual environment (the world and objects), they may need access to related information about the objects or world. This abstract or symbolic information could include text, links, numbers, graphical-plots, and audio/video annotations. Thus, the design challenges of IRVEs are particularly relevant to Computer Aided Design (CAD), Computer Aided Manufacturing (CAM), virtual exhibits, and scientific and military simulation applications. For example, take cases in the domain of chemistry, chemical engineering, and cheminformatics. Chemical data is multi-faceted and heterogeneous: structural, nominal, ordinal, and quantitative data (such as their physical characteristics) are all associated to molecules and their constituent atoms and bonds.

For abstract data, established information visualization techniques are useful to show different qualities and relationships in the dataset [4,5]. In chemistry, there is a growing body of data on molecular compounds: their physical structure and composition, their physico-chemical properties, and the properties of their constituent parts. When considering information *about* a molecule or its parts, such established visualization techniques can be used. For example, names and annotations can be displayed as textual tables, spectral data with multi-dimensional plots, and classifications with tree diagrams. In these abstract contexts, however, inherently spatial attributes of the data (such as the physical structural of atoms and bonds in a molecule) are difficult to understand.

Spatial data may be best portrayed and understood in 3D interactive or immersive views. This is apparent in the success of virtual environment platforms for architectural design and analysis, civic planning, geology, and medicine. Additionally, it has been shown that conceptual learning can be aided by features of VEs such as: their three-dimensional perceptual aspect, their support for users to change their frames of reference, and the inclusion of multi-sensory cues [6].

Typically in the literature, visualizations are described and categorized per-user-task such as exploring, finding, comparing, and recognizing patterns. Such tasks have shown to be well supported through the use of tightly-coupled, multiple-view visualization techniques [7,8]. Since these tasks are common in information-rich virtual environments as well, we believe that the qualities of parallelism of display and coordination of views can also help users of IRVEs. This strategy can give users easier, integrated access to information and help them to generate insight through stronger mental associations between physical and abstract information while preserving mental models of each type of information.

This paper explores the use of multiple-views techniques to link structural visualizations in a virtual environment with visualizations of abstract data about those structures and their constituent parts. We demonstrate the embedding of an information visualization application in a virtual environment and explore the coordination mechanisms between them. We describe the supporting architecture of our system, which treats the CAVE or other 3D viewer as a component of generalized capability. Finally, we evaluate the system's usability and report issues and lessons learned for future IRVE system design.

2. RELATED WORK

While prior work has elucidated design criteria for 2D or 3D information visualizations, little of this work addresses the combination of *embedded*, *coordinated* 2D visualizations in an immersive environment. A challenge of this project is how software and communication architectures can work together to support coordinated displays and interactions across rendered dimensions. Our work extends previous research by having 2D and 3D views of a complex data set linked across web based Snap-Together Visualization system [9] and the DIVERSE virtual reality software platform [10]

2.1 Information Visualization and Multiple Views

A growing body of work is leveraging object-oriented software design to provide users with multiple linked views or renderings of the data. Roberts [8] and Boukelifa et al. [11] have described additional models for coordinating multiple views for exploratory visualization including 2D and 3D views. In Roberts' Waltz system for example, multiform 2D and 3D visualizations of data are displayed and coordinated as users explore sets and subsets of the data.

We have also described a taxonomy of tightly-coupled views [12] which reviews systems and experimental evidence of advantages including significant speed up on overview+detail tasks. These visualizations are coordinated by simple events such as*:* 1. Selecting items ↔ Selecting items, 2. Navigating views ↔ Navigating views, and 3. Selecting items ↔ Navigating views, for example. The 'Visualization Schema' approach allows users to build their own coordinated visualizations [9]. We would like to extend this concept to virtual environment design so that embedded information and interfaces inside the environment can be customized and composed in a structured way.

Baldonado, Woodruff, and Kuchinsky [13] have proposed guidelines for building multiple view visualizations. They claim four criteria regarding how to choose multiple views: diversity, complementarity, parsimony, and decomposition. They also put forward four criteria for presentation and interaction design: space/time resource optimization, self-evidence, consistency, and attention management. Recent empirical research supports these guidelines[14] and methodologies for designing multiple views should evaluate their design according to these criteria. While these guidelines are well-formulated for 2D media, none have been critically evaluated in the context of 3D worlds as we propose.

2.2 Immersion and Virtual Environments

Our DIVERSE application supports both 3D visualization on the desktop and 3D immersive display in the CAVE [15]. Our motivation for immersive visualization of molecular structure is supported by previous research. According to Ware and Franck [16], the graph that can be understood with a head-coupled stereo view is three times as large as the 2D graph for any given error rate. Also, Datey [17] shows that visualization of inherently spatial data proves better in immersive VEs. Because our molecular data is both graphical and spatial in nature, immersive environments seem ideal.

Dykstra [18] was the first to demonstrate how X11 windows could be embedded and rendered within virtual environments, and our work extends this concept. While Plumlee and Ware [19] have used multiple embedded views and frames of reference for the navigation of large-scale virtual environments, their augmenting views only provide additional spatial cues or alternative views of the perceptual world. Finally, Bowman et al [3] have implemented and evaluated an information-rich 'Virtual Venue' with a number of features that are common to our project such as navigation and information retrieval through menus and spatial hyperlinks.

The use of menus in immersive systems has also been investigated, showing a good translation of the 2D metaphor to 3D environments. For example, Bowman and Wingrave have compared Pinch Glove, floating menu, and pen and tablet menu systems. While pen and tablet interaction was significantly faster, but users preferred the Pinch Glove system [20]. Design principles for interaction techniques have been described in terms of performance and naturalism [21]. More work is needed however to determine how these techniques can be applied to embedded, coordinated visualizations and if naturalism and performance are affected by issues of display form, interactive context, and their different combinations.

3 DESIGN

This paper describes our work to address the Coordinated View problem in the context of a molecular visualization application. We wanted to develop a system for integrating multiple views of heterogeneous physical and abstract data and identify usability issues with these displays in immersive environments. While this framework for coordinated viewing is applicable to a variety of data domains such as medicine, engineering, and architecture, we chose to use a set of Chemical Markup Language (CML) files since we had some experience with the language and the variety of data captured in the files exemplifies the combination of perceptual and abstract information types.

Tasks and scenarios we wanted to address concern how well users can locate, relate, and understand information across the abstract and perceptual visualizations. Some example tasks a researcher or analyst may ask our system to support are as follows:

- **Exploring** - Load molecules into the 3D View. What are some structural or geometric features of *this* molecule? What are some characteristics of *this* molecule (boiling point, melting point, etc)? How about *this* atom (radius, weight, number)?
- **Finding** - How many atoms are there in Caffeine? What are the bond types and lengths?
- **Comparing** - Which compound has more double bonds, Caffeine or Histamine? Which has more Nitrogen atoms? Which is heavier?
- **Pattern Recognition** – What are the similarities and differences between Caffeine and Histamine molecules?

Our system uses the DIVERSE toolkit [10] and Snap-Together Visualization [9] for integrated visualization tasks such as overview, navigation, details-on-demand, and brushing-and-linking selection. It can be run on a desktop with 2D and 3D views in separate windows, but we are more interested in the use of coordinated 2D visualizations inside an immersive 3D world such as the CAVE. In a CAVE, input and output requirements are different. We demonstrate a system where users can visualize and interact with multiple information types by way of a 'Hanging Picture' window superimposed on the immersive virtual world (Figure 1).

There are a number of possibilities as to how abstract information is related to the perceptual information in an IRVE [1, 22]. This project explores the multiple views part of the IRVE design space. From an IRVE information design perspective, we first enumerate the visual layout of abstract information in the virtual environment- we must determine the *location* of the information, decide on the *association*s between the perceptual and abstract information, and appropriate the *types*, *aggregation*, and *density* of abstract information based on screen space, the visual field, and users' tasks. From an IRVE interaction design perspective, users may index into the perceptual information through the abstract information and vice versa.

3.1 IRVE Information Design

We use the DIVERSE virtual reality toolkit to display inherently spatial data such as the 3D molecular structure. A considerable amount of work has been done in the field of visualizing chemical compounds with several types of visualizations implemented in 3D and immersive environments. Our project combines a web-based visualization system with the 3D immersive view that the CAVE provides. 'A Functional Framework for Web-Based Information Visualization Systems.' [23] addresses 3D molecular visualization applications and gives a good overview of the ways molecules can be visualized; our DIVERSE application, s_AtomView, uses the 'ball and stick' 3D display for atoms and bonds in molecules.

There are at least four possibilities for *locating* abstract information into the visual field. They are world-fixed, display-fixed, user-fixed, and view-fixed locations [1,24]. Information may be associated to a particular object in the world, which is termed as 'object-fixed'. Alternatively the abstract information may be associated to a location in the world, which is termed 'world-fixed'. If the annotation travels with the user regardless of their navigational actions, this is classified as 'user-fixed'; if persistently located on the display, it is termed 'display-fixed'.

Figure 1. CAVE user navigates to an atom and its bonds, which are highlighted as a result of selection in the 2D Hanging Picture that is hung on the right wall

In order to give users simultaneous visual access to the perceptual and abstract information, we demonstrate what we call 'The Hanging Picture Metaphor'. In this design, the Snap application window is 'hung' on a wall of the CAVE. The contents of the picture are the 2D visualization components set up through Snap's visualization schema. The Hanging Picture is different from common Heads-Up-Displays (HUDs) in that it is a separate, opaque application and does not reside within the scenegraph; it is a display-fixed location. This is also true if the Snap2Diverse software is run in separate windows on a desktop.

The *association* dimension of IRVE layout defines the interrelationship between the perceptual and abstract information. Various layout techniques in two-dimensional (2D) space have been proposed considering usability and human perceptual and cognitive issues. For example, the Gestalt principles should be applied to IRVE design to evaluate the configural properties of visual information: connectedness, proximity, common region, similarity, and common fate (most recently summarized by Ware [25]). The association of information in the Hanging Picture can be described as 'visually implicit' since its display is not localized in the environment and association between the multiple views is based on brushing and linking.

The multiple views approach is advantageous because there may be a variety of abstract *information types* that are related to a given perceptual data item. For each of these types, there are already effective 2D visualization techniques that we want to use. The Snap event and component architecture fills this requirement nicely, since multiple multiform visualizations can be displayed and coordinated. Snap is a web-based interface for creating customized, coordinated, multiple-view visualizations. Through web pages and Java applets, Snap provides users with the ability to build layouts of multiple visualizations of data in a database with components such as tables, scatter plots, and various charts and graphs. Users can interactively combine visualization components and specify coordinations between the components for selection, navigation, or re-querying. Using the concept of a 'visualization schema', Snap allows users to coordinate visualizations in ways unforeseen by the original developers. We decided to use Snap because of this end-user flexibility and the ability for developers to define new visualization components.

Lastly, the *density* of layout is a visuo-spatial measure of the amount of information we can display in one field of view (a frame). This is hard to measure quantitatively, but involves the proportioning of the visual field between 3D objects or areas and their labels to other 3D objects and areas (and their labels). Given a display's size and resolution plus legibility and readability constraints for textual information, there is only a certain density that can be supported on any given display platform. Layout density impacts things like crowding, occlusion, and distraction. Because the information in the Hanging Picture is highly aggregated (into one application window), there is little relative density in the Snap2Diverse IRVE layout.

3.2 IRVE Interaction Design

A principal advantage of Snap and the Hanging Picture is that the picture is customizable and interactive. Users can compose tightly coupled visualization components and coordinate selection events for brushing and linking interaction. When a CAVE Adapter is connected into the Snap visualization schema, load and select events can be routed to the DIVERSE system and the 3D objects corresponding to that selection are loaded or highlighted as shown in Figures 1 and 2.

The brushing and linking interaction between perceptual and abstract information allows users to explore and search the data space by way of the abstract information or the perceptual information. The result of indexing into any of these views is a coordinated selection event that highlights the appropriate object and attributes in all other active views. In Snap2Diverse, brushing and linking can be used to relate or compare the structural, physical, and chemical properties of molecules, atoms, or bonds.

Coordinating 2D and 3D views in a virtual environment not only requires the sharing of addressable data objects and event communication across the applications but also special interaction facilities for immersive displays such as our CAVE. User input in CAVE systems is typically through the use of a 6 degree-of-freedom tracked 'wand' which has a number of buttons and a thumb-size joystick. We used the XWand software developed at Virginia Tech to manage navigation interactions in the virtual environment and mouse emulation for selection and dragging in the Hanging Picture.

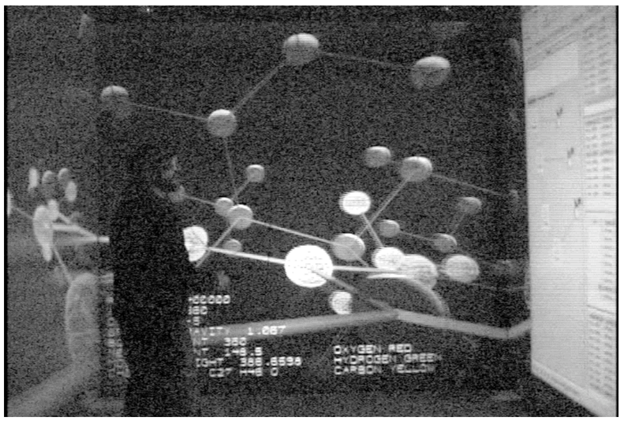

Figure 2. CAVE user explores the properties and relationships of Carbon atoms in a Histamine molecule

4. IMPLEMENTATION

The principal technologies used in our implementation are shown in Figure 3 and described below.

4.1 Data Sources

Chemical Markup Language is a new approach to managing molecular information [26,27]. It has a large scope as it covers disciplines from macromolecular sequences to inorganic molecules and quantum chemistry. CML is new in bringing the power of XML to the management of chemical information - its design supports interoperability with the XML family of tools and protocols [28]. CML contains a number of kinds of information about a particular compound, from its physical atomic structure and elemental makeup to its water solubility, melting point, atomic weight, and various spectral descriptions. These are manifested by a variety of datatypes in tags describing structural, numerical, and metadata about the chemistry of the molecule. CML provides a base functionality for atomic, molecular, and crystallographic information and allows extensibility for other chemical applications. The developers of CML have provided a DTD, Schema, and an API toolkit (CMLDOM). In addition, they provide Jumbo, a Java-based application to load and view a number of chemical formats in CML (CIF, MDL, MOL2, PDB, XYZ JMOL) and write them out to any of those formats.

Given the capability and flexibility of CML to describe molecular information and the wide support for XML tools, we chose to source our data in this format. Because CML is a dialect of XML, we are able to use Extensible Stylesheets (XSLT) to transform the single source data file to multiple representations [29]. Currently, Snap requires its source data to be a relational database. Therefore we had to generate normalized, relational tables from the hierarchical CML data source. Additionally, because the DIVERSE AtomView application was written to load files into the 3D world and had little database capability, we needed to generate simple X3D files containing the molecules' geometry, atoms, and bonds and some basic text information. In order to accomplish this, we built a simple Java tool to easily transform different source files with different XSLT stylesheets. For each of our destination platforms, we wrote a set of XSLT files specifying the proper attributes of the output method, encoding, media-type, and cdata-section-elements, and the DOCTYPE system for our result document.

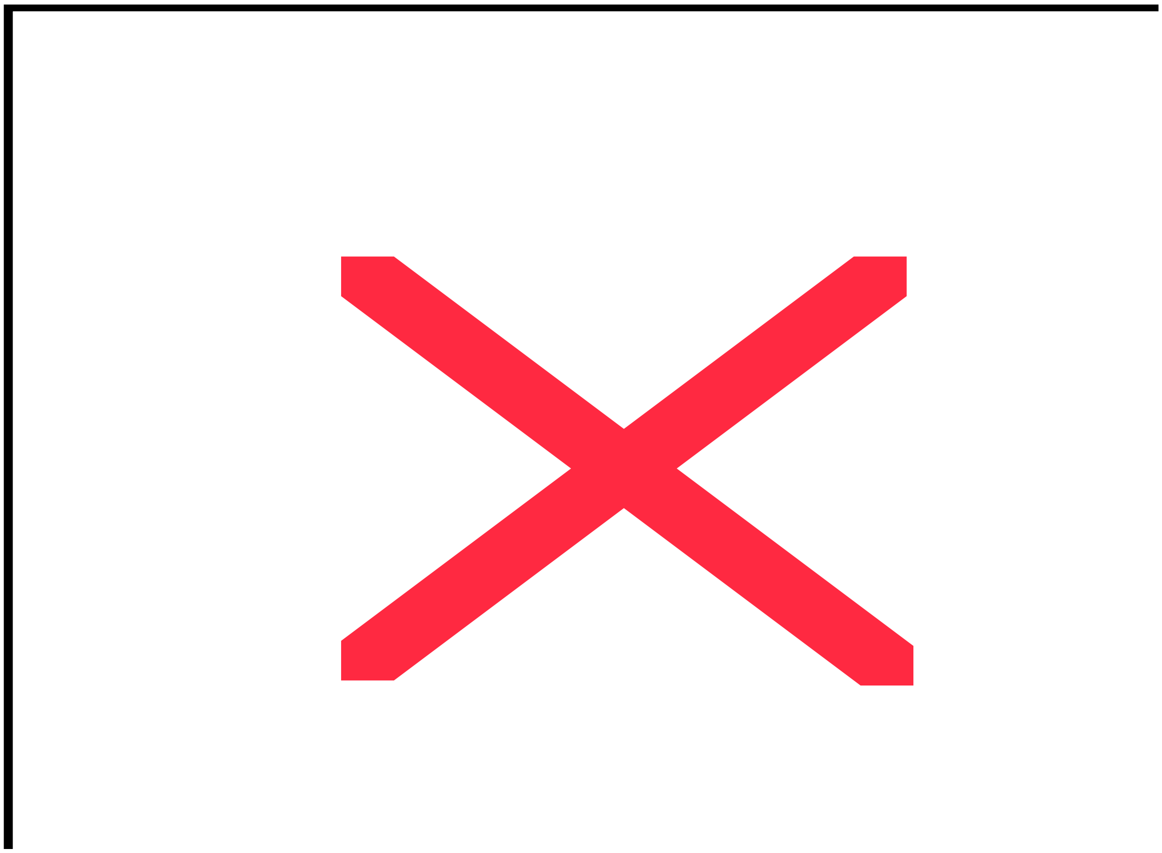

Figure 3. System Architecture

We maintained consistency of the data items by using the CML id attribute to guarantee uniqueness of the elements across representations. Building the Snap relational database from a hierarchical data structure presented some challenges. First, we examined the semantics of the data structure in the CML file and determined that multiple tables were needed such as: molecule, atom, bond, atomic_constants, and spectral data. For each table in the database, we created an XSLT stylesheet to transform the appropriate CML tags to a comma-separated file (csv), which could be loaded into MS Access and then into SQLServer.

While building the database, we discovered some limitations of the relational data model that have to do with many-to-many relationships and join operations. Consider atoms and bonds for example; a bond connects two atoms but from our available data, it does not have a directionality associated with it. For a Snap event to connect an atom and its bonds or a bond and its atoms, we had to add an intermediary, redundant 'bond2way' table even though it makes no sense from the CML data model to claim that one is the start_atom and one is the end_atom.

4.2 Extensible 3D (X3D)

The Web3D Consortium's next-generation successor to VRML is X3D, which, like XML, moves beyond just specifying a file format or a language like VRML or HTML. It is a set of objects and interfaces for interactive 3D Virtual Environments with bindings defined for multiple profiles and encodings and collected under a standard API [30]. The X3D specification describes the abstract properties of a directed, acyclic scenegraph, which can be defined by an XML binding using DTDs and Schema. In addition, rather than defining a monolithic standard, the X3D specification is modularized into components that make up 'Profiles'. Profiles are specific sets of functionality designed to address different application domains from simple geometry interchange or interaction for mobile devices and thin clients to the more full-blown capabilities of graphical workstations and immersive computing platforms.

The X3D Task Group has provided a DTD, Schema, an interactive editor, and a set of XSLT and conversion tools for working with X3D and VRML97. While the structural geometry of the molecule could be described in X3D simply as primitives conforming to the Interchange Profile (Sphere, IndexedLineSet), our X3D data files for DIVERSE used high-level markup (Prototype tags) to describe the data in the scenegraph. This way, the displayed form of an atom or bond could be customized by the application (atoms as a Sphere, bonds as lines or cylinders).

4.3 Snap-Together Visualization

Snap provides an interface for developers to build their own Snap Adapters to custom visualization components. We take advantage of this capability by defining the CAVE Adapter, a set of classes that process events from Snap and communicate them to the remote DIVERSE visualization. Because Snap currently has no event mechanism to declare from which visualization component an event originated, we built the adapter to actually manifest three adapters in the visualization schema: one for a molecule-visualization event, one for an atom visualization event, and one for a bond-visualization event. The connectivity of coordinating events in our application is shown in Figure 4.

In order to embed our 2D Snap visualizations in the CAVE, we initialize our DIVERSE application (next section) and export the display of a remote machine Linux machine with Mozilla and Java to the CAVE wall. The CAVE at Virginia Tech runs with 3 walls and a floor projection. We then run Mozilla on that remote machine and connect to our online Snap build and Molecules database. At this point, the browser window with the Snap applet is live and 'hung' on one wall of the CAVE. Since the Snap window is running from a remote Xserver and exported to a CAVE display, we can hang the picture anywhere on either the left or the right wall.

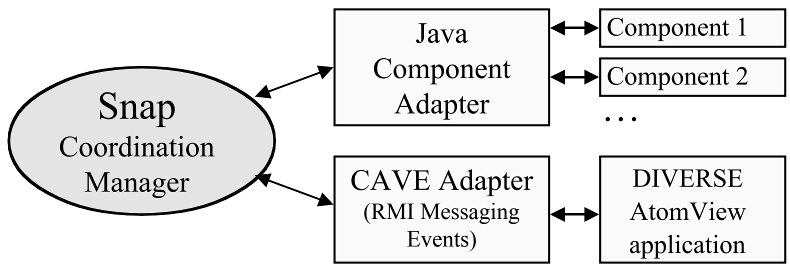

Figure 4. Event schematic for multiple views

In our usability evaluation, we hung the Snap window aligned to the top-left of the right wall. Users can then connect their Snap visualization components and load, sort, and select data records of interest. As we have mentioned, Snap allows users to build their own coordinated multiple-view visualization schemas. This gives great flexibility for customizing the layout of data displays and interactions.

Figure 5 shows a typical Snap window setup connected to our molecules database and coordinated with the Cave Adapters. In this screen shot, the hierarchy of molecular data tables is established and linked through brushing event coordinations (Select <-> Select in Snap terminology). The atom table is linked to a scatter plot of atomic number versus atomic radius. For the case of ultra-violet (UV), infrared (IR), and Mass spectrum data, we setup Select <-> Load event coordinations to graphing components. This means that when a user has selected a molecule to examine, only the spectrum data for that molecule is loaded and rendered. In Figure 5 for example, the user has selected a Nitrogen atom from the molecule caffeine and the IR and UV spectrum response for the caffeine molecule is loaded into the bottom-left and bottom-right Scatter plots respectively.

4.4 DIVERSE and AtomView

DIVERSE is a software toolkit for building portable virtual environment applications developed by the University Visualization and Animation Group at Virginia Tech. Our VE application is written for DIVERSE and extends AtomView, a molecular visualization tool for materials scientists also developed at Virginia Tech. DIVERSE provides some powerful advantages:

- A common user interface to interactive graphics and/or VE programs. Using DIVERSE the same program can be run on CAVE™, ImmersaDesk™, HMD (head mounted display), desktop and laptop without modification.
- A common API to VE oriented hardware such as trackers, wands, joysticks, and motion bases.
- A "remote shared memory" facility allows data from hardware or computation to be asynchronously shared between both local and remote processes

When the application starts, it reads in constants for the different elements, which are used to scale the atom sizes based on atomic radius. Next, geodes are created for each possible color, highlighted and un-highlighted, for the atoms and bonds. These geodes are linked to multiple atoms and bonds that are displayed in the application as spheres or cylinders. The program now waits for messages from the Snap side.

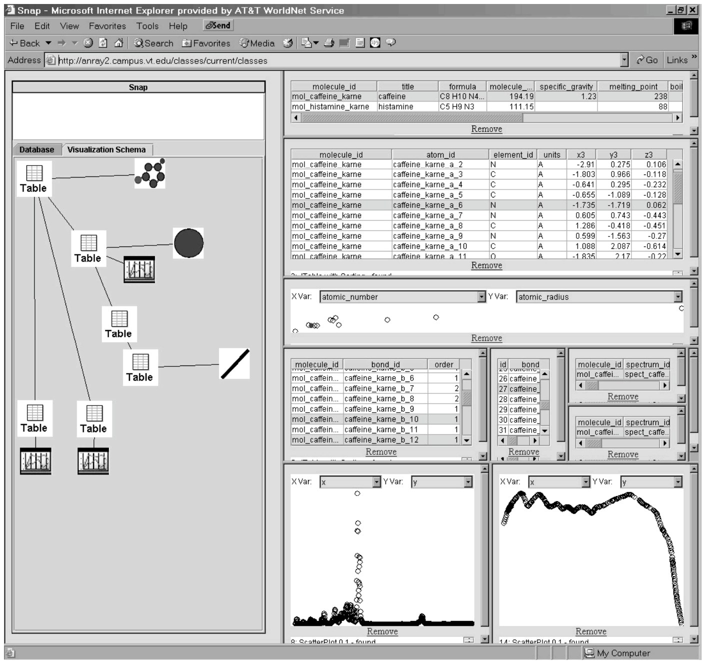

Figure 5. A sample Hanging Picture: a Snap visualization schema coordinated with the Cave Adapters. A Nitrogen atom of the Caffeine molecule is selected.

When a molecule message is received, the program reads the molecule name and appends the file suffix to read the atom, bond, and molecule description text data from a local X3D file. This molecule message also results in reading the molecule's corresponding color data from a separate file. This color data allows the program to link atoms and bonds to their corresponding geode. Based on the location of other molecules and the base location of the atom, atoms are added to the world. Bonds use the same information as atoms to find their correct position, but also require vector calculations to line up between atoms.

Now that a molecule is added, the program waits for more messages. If another molecule message is received, the program removes the molecule if it is already in the program and visible. Otherwise, it adds the molecule as before. If an atom or bond message is received, the program searches the corresponding molecule for the object and highlights or un-highlights based on the current state. Molecule description information can also be displayed in a Heads-Up Display window, and this information changes when you move from molecule to molecule (see Figures 1, 2, and 6).

Selection in the VE is accomplished using simple ray-casting and a wand button. Upon selection in the 3D world, the corresponding records in the Hanging Picture are highlighted. Future work on the DIVERSE side could include adding element letters inside each atom so they can easily be identified, sliders to change the transparency of the atom, and commands to allow easy re-centering and movement between molecules (see Polys 2003 [29]).

4.5 XWand

XWand is a program that allows you to use an input device such as a wand to start, stop, and manipulate any XWindows application. XWand works by using the DIVERSE Toolkit (DTK) to obtain input from devices in an immersive environment such as an iDesk or CAVE. It works by using XTest extensions in conjunction with input from DTK. In addition to the XWand program, there is also an XWand DSO that, when loaded into a DIVERSE application, can stop and start the navigation for the currently running application, giving the XWand program control over the navigation events. We used this program to allow users to toggle their interactions between navigation in the CAVE environment and selection in the 2D applet view.

4.6 Coordination

The Diverse ToolKit (DTK) 2.0 handles messages through its shared memory component. Snap, on the other hand, handles inter-process communication within the JVM. We wanted to use both of these systems, but they do not mesh well together. If both systems were implemented in Java it would be easier, but DTK is a C++ toolkit. Therefore we wrote a Remote Method Invocation (RMI) wrapper for messaging between the applications. We send select events based on molecule, atom, and bond IDs between Snap and DTK. This allows users to index into the data from either direction.

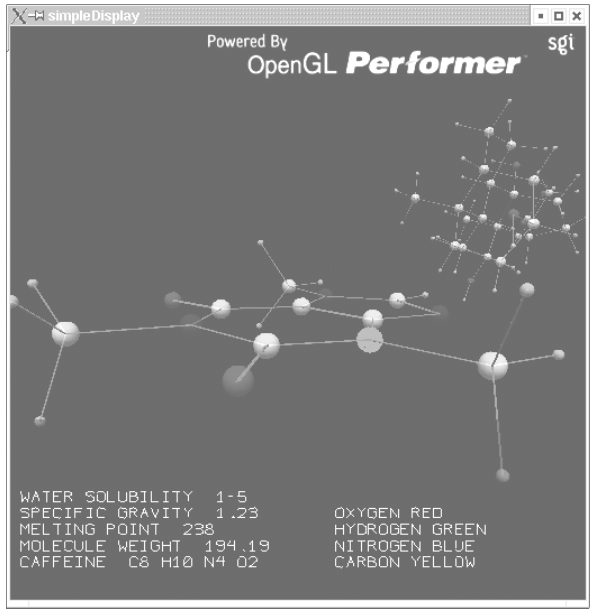

Figure 6. Two X3D molecules on a DIVERSE desktop platform. The Heads-Up-Display shows information relating to the nearest molecule. A Nitrogen atom of Caffeine is highlighted as a result of selection in Snap.

DTK then uses the primary keys sent by Snap and further processes those. We implemented communication in Snap by using three specially-developed adapters. These adapters receive Snap events and then use Java RMI to send the information back to a server that we set up to receive these RMI commands. By using the networking features of DTK, we were able to then connect the CAVE to this computer and the CAVE would receive the messages from the Snap server. In the future, it may be more beneficial to come up with a consolidated method of having one intelligent adapter that can send and receive Snap events from DTK. This would probably be implemented with some form of CORBA or similar technology.

5 USABILITY EVALUATION

5.1 Procedure

The team members discussed possible usability issues and the representative tasks to test different aspects of the system. Subjects were chosen from a cross-section of people: an undergraduate chemistry student, a graduate computer science student, a materials scientist, and virtual reality experts from within our lab.
The specific aspects we wanted to evaluate were:

- Viability of a visualization involving simultaneous, coordinated 2D and 3D displays
- User preference based on nature of data, i.e. whether users choose most appropriate visualizations for different types of data.
- Effectiveness of 3D to visualize inherently spatial data.
- Use of a novel interaction system (XWand) for interaction with the 2D display in a 3D immersive environment.

The format followed for the usability study was task and response. The subjects were given a set of tasks to be performed one by one and their feedback was noted. Eight tasks were formulated that can be classified into four categories: exploration tasks, finding tasks, pattern recognition tasks, and comparison tasks (see Sec. 3). Exploration tasks involved loading and describing features of various chemical components. The finding tasks involved getting the number of atoms or bonds in a molecule or finding a specific attribute of an atom, bond or molecule. The pattern recognition and comparison tasks asked users to detect and describe similarities and differences between two molecules such as their size, molecular weight, and shape. We used the molecules caffeine and histamine for the evaluations.

The step-by-step procedure was as follows:

- Introduction: The subjects were introduced to the system and the scope and limitations of the system were explained. The XWand interaction techniques were demonstrated, and the procedure was described. The subjects were asked to think aloud during the tasks.

- Tasks: The tasks were read out for the subject and their subjective feedback for each task was noted. We also noted down their actions such as where they search for particular information (in 2D or 3D), the problems or discomforts they face with the interaction techniques, etc.
- Closing questionnaire: At the end of the usability study each user was given a closing questionnaire to reflect on their opinion about this system.

5.2 Results

The results of the usability evaluation were obtained from user observation and the feedback questionnaire. They consist of usability measures, technical deficiencies, and suggestions by subjects. Usability measures we evaluated included: the time to understand the basic concept of coordinated 2D and 3D visualizations, the learning time for system interaction, and the degree to which a new user is overwhelmed by the CAVE.

In the evaluations, the location, size, contents, and layout of the visualization components were fixed for the users. New users experienced a high cognitive load just familiarizing themselves with the meanings of the contents of the Hanging Picture. This may be the result of the design of the abstract information visualizations since the Snap information displays provided much more information and affordances than needed to complete the specific tasks. That is, for the given tasks, the information the system actually provided exceeded the information required to complete that task, thus overloading the user. If users were chemistry experts or more familiar with the Snap system, they may have had a more intimate understanding of the contents of the Hanging Picture.

The tasks (i.e. Sec. 3) were designed so that users would have to answer a question about spatial properties based on some abstract information criteria or vice versa. In addition, there were questions that could be answered by either perceptual or abstract sources. In most cases, users chose suitable visualizations to recover the information required for the finding and comparing tasks. This suggests that users were capable of interacting with and comprehending both the abstract and perceptual information via our multiple views IRVE design. If the task was an exploration task or pattern recognition task and could be accomplished by referring to either the perceptual or abstract information, nearly all users resorted to indexing via the perceptual (spatial) information.

Learning time for the brushing interaction was surprisingly low for both VR novices and experts. The use of the wand was initially confusing for novice subjects, but after a few minutes they could fluently use the wand for: navigating by flying (thumb joystick), toggling between the navigation and selection mode (button 1), and selecting a Snap information item (thumb joystick and button 2). The visually implicit association between perceptual and abstract information (coordinated highlighting via selection) was established between the multiple views and sufficient for completion of all the tasks.

One important feature suggested by the subjects was to reduce the size of the 2D browser window or put it on some hand-held device like a tablet in order to avoid occlusion of the virtual world. Similarly, a pen and tablet interface might be faster for interaction than the wand. The closing questionnaire showed that the subjects considered this system a better learning device than a textbook or 2D diagram and the wand was fairly intuitive as an interaction device. However, the opinion was divided over whether the wand was a hindrance in using the 2D Snap window.

Some technical shortcomings of the implementation became apparent during the study. First, there was a decrease in the 3D navigation speed as users repeatedly toggled the wand (for interaction with the Hanging Picture). Second, selecting from the 'Hanging Picture' wall was slow: the responsiveness of the pointer when moving over the Hanging Picture was tedious. In addition, our prototype had no routines to automatically reset the Viewpoint to a 3D molecular structure in the space if reference gets lost (if the molecules were too far away or the user became disoriented); this is a crucial usability issue in VEs.

After summarizing the results and improving the initial build, we produced an informational video about the project details and filmed it in the CAVE (http://infovis.cs.vt.edu/IRVE). Based in our usability results, we have to consider our system as tested to be high-threshold, high-ceiling in terms of learnability and functionality. The issues reported are important considerations for future work in the design of Information-Rich Virtual Environments.

6 CONCLUSIONS AND FUTURE WORK

The Snap2Diverse system has shown that there are three crucial issues in the design of IRVEs. First, we need to design better data models that integrate perceptual and abstract information. Second, the transformations that map that information to VEs and InfoVis applications must be carefully considered. Third, we need a flexible but structured way to support the display and interaction coordinations between the VE and InfoVis applications. Snap's event-based coordination mechanism has proven a useful system to integrate abstract and spatial visualization applications.

Our current multiple views implementation makes use of the wand and the Hanging Picture to interact with perceptual and abstract information in the same environment. In terms of the IRVE design space, Snap2Diverse can be characterized as: a display-fixed location, low-density layout with visually implicit association of aggregated abstract information of multiple types. Another interesting design option to explore are the tradeoffs involved in putting the Snap display and interaction window on a hand-held tablet surface. This last possibility raises the question of how to better integrate external applications into IRVEs. The trend toward event-based, Model-View-Controller interfaces could bear this out. For example, the principles that make the Hanging Picture work could be extended to the generalized notion of an 'application texture'. In this approach, the windowing system would manage the rendering and pointer events for an application mapped to some geometry in the world. The X3D Specification Working Group is currently developing a 'Compositing Component', which may address this important functionality.

For our system to be more successful, more virtual environment interaction techniques should be implemented and evaluated. For example, in our prototype version, if the user became lost in the 3D world, there was no way to reset the viewpoint except to reload the application, which was not a good option. Flexible interface widgets and windows (such as VEWL components [31]) could be added to manage and expand more system control functionality. Additional 3D interaction techniques for navigation and selection should also be explored including picking touch, laser pointer, and spotlight techniques [32,33]. Future work with Snap could be to relax its data model in order to better deal with hierarchical sources, as well as possibly specifying the component of origin in the SnapEvent class.

We have demonstrated a heterogeneous system for embedding interactive, user-defined 2D visualizations inside 3D virtual environments and coordinating them across a network. The architecture we describe is flexible for linking Snap with DIVERSE and could be applied to any number of data domains. In terms of our chemical visualization and analysis application, Chemical Markup Language and XSLT give us great flexibility in the loading of chemical data into the visualization pipeline from different formats. We also believe this approach could be applied to embed and coordinate any XML data in such Information-Rich Virtual Environments. This work contributes to the field by implementing and assessing an Information-Rich Virtual Environment design for multiple, coordinated views of perceptual and abstract data. Our initial evaluation of this system identifies critical usability concerns when coupling 2D information visualizations with 3D immersive virtual environments.

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