

CCSC

Consortium for Computing Sciences in Colleges

Southeastern Region

**31st
Annual
Southeastern
Conference**

**Student Research
Contest**

**Extended
Abstracts**

**November 3 and 4, 2017
Furman University
Greenville, South Carolina**

Table of Contents

Algorithmic Detection of Emotion for Emotional Disabilities.....	3
<i>Alexandra Meads</i> <i>Elon University</i>	
Modelling Protostellar Disk Formation with C++.....	6
<i>Austin Bane</i> <i>Roanoke College</i>	
Term Extraction from Historical Articles using the Stanford Parser.....	8
<i>Drew Luther</i> <i>Roanoke College</i>	
Visualizing Molecules Using Augmented Reality and Image Recognition.....	10
<i>Mike Deiters and Kevin Stevens</i> <i>Georgia Gwinnett College</i>	
MR. Mol: Mixed Reality Molecule.....	12
<i>Robert Alexander, Matthew Camp, Pedro Garcia, Anastasiya Golovan,</i> <i>Jacob Piazza, and GinaAnn Rosbury</i> <i>Georgia Gwinnett College</i>	

Algorithmic Detection of Emotion for Emotional Disabilities

Alexandra Meads, Elon University

Mentor: Dr. Shannon Duvall

ABSTRACT

Emotion-recognition technology is an emerging field that has been under-utilized for people with emotional disabilities. This technology has largely been explored and developed around typical emotional expression as well as facial recognition. These applications are therefore not applicable to people who emote atypically or to situations where a user can behave naturally instead of positioning themselves in front of a camera. In this research, we present an implementation of the k-nearest neighbor algorithm, which takes the joint angles of emotional body postures to learn and recognize a user's custom emotional body expression. This can then be utilized in interactive spaces to assist people with emotional disabilities.

INTRODUCTION

Assistive technology is a varied field which serves people with a wide range of disabilities. However, this field is lacking when it comes to assisting people with emotional disabilities. Affective computing can be and is applied to any and all physiological aspects available, yet this research is frequently based on *typical* emotional expression. People with emotional disabilities do not always emote typically, rendering much of what is available inapplicable to them. Additionally, much of emotion recognition technology relies on a user's facial expression. This does not necessarily exclude use by those with emotional disabilities, but it does limit use to a specific setup, as opposed to emotion recognition in a more natural environment. Consider instead a user interacting naturally in their home or school, and when the person experiences distress or self-harm behaviors, the lights and sounds of the room could change to accommodate them. This research could contribute to the creation of such an interactive space designed specifically with people with emotional disabilities in mind. [1]

Currently, most interactive systems are expensive and located in public places, like museums, but the benefits of the proposed system would come from it being in a home or similarly-used environment. The proposed system would tentatively use an Xbox Kinect as its camera source, which can interpolate unseen joint locations. This technology is relatively inexpensive as well as portable. Furthermore, the proposed application's algorithm would be trained on user-submitted data, allowing for initial labelling of postures with their associated emotions for that specific user. With this training data submitted, the user's body postures obtained via natural behavior in view of the Kinect could then algorithmically be mapped to a corresponding emotional state of anger, disgust, fear, joy, neutrality, sadness, or surprise. People with emotional disabilities could have an affordable, portable, and most importantly, customizable interactive space in their own homes to assist with their emotional needs.

OTHER ALGORITHMS AND METHODS

Before selecting the K-nearest neighbor algorithm, we entertained the use of a few other machine learning algorithms for this research. We looked into using random forest classifiers, support vector machines, and deep learning. Random forest classifiers were considered for their ability to avoid high variance and high bias, while support vector machines generally create excellent decision boundaries.

Deep learning has proved superior in many cases to traditional machine learning approaches. The prohibitive element with these algorithms was that they require large amounts of data to ensure accuracy. Acquiring so much data in order to test this idea would not have been possible unless perhaps we collected data from typically-developing people, which was not feasible in addition to missing the point of the research and likely not being applicable to our intended user base.

Something else considered during this process was the use of static body posture mapping. Previous research has been conducted on affective body gesture analysis in videos, supporting the viability of modelling gestures from spatial-temporal features and the possibility of connecting those gestures with emotional states [3]. Static body posture mapping could work for connecting certain postures with emotions, but our previous work found people will not always make those postures simply because they are feeling those emotions. This approach also lacked the proper data of atypically developing people.

K-NEAREST NEIGHBOR

After eliminating random forest classifiers, support vector machines, deep learning, and static body posture mapping, we decided to attempt this study using the k-nearest neighbor algorithm (KNN). This algorithm has several attributes that make it ideal for our proposed technology. It is a fairly straightforward algorithm; given a few labelled data points, it labels a new point's position based on its closest calculated distance to another point. More importantly than its simplicity, this algorithm can be implemented with a small amount of data, while still being fairly accurate.

The data-gathering aspect associated with KNN is significant to this research in particular. [2] The fact that we can test it using a small amount of data simulates a real user situation wherein someone might label a mere handful of emotional posture images to setup the system for personal use. KNN, like other machine learning algorithms, gets better over time the more data that is introduced to it. This will allow the system to be gradually tailored to an individual's emotional expression. These aspects of the KNN algorithm can allow for a system customized to the individual without them having to do too much setup to begin using said system.

PROCESS

To test the viability of our proposed solution, we implemented k-nearest neighbor using pre-existing calculated joint angle data from the Emotional Body Motion Database (<http://ebmdb.tuebingen.mpg.de/>), and then the program was tested programmatically for accuracy. For data points, with (Tag, Real) representing their emotion tagged via the algorithm and their actual emotion respectively, precision and recall were calculated via the average of each emotion after using the following formulas:

Precision for emotion X = # tags of (X,X) / # tags of (X,_)

Recall for emotion X = # tags of (X,X) / # tags of (_,X)

With no adjustments to the algorithm or joint angle data, this approach has approximately 86% precision and recall accuracy. Through further testing of various data configurations, we will attempt to answer two questions and find the optimal design: how much initial data is needed for an acceptable level of accuracy? And which joint or angle combinations yield the most accurate results? It will be important to know how much initial data a user would need to submit in order for the program to accurately assess

their emotional state. Furthermore, it is possible only certain joints or joint angles hold significance for emotional postures, and certain joints or joint angles might interfere with accurate assessment. If that is the case, we need to determine which combinations to use.

After fine-tuning the algorithm, we would potentially try it out with user data from a member of our target demographic. This would allow for a realistic implementation of our program to assess the accuracy when applied to a person with atypical emotional expression. Taking this next step is important not only for us to test the accuracy of our application, but also eventually for someone else to test the usability of the project.

REFERENCES

- [1] Cearreta, I., López, J.M., López de Ipiña, K., Garay, N., Hernández, C., Graña, M. 2007. A study of the state of the art of affective computing in ambient intelligence environments. *Interacción 2007 (VIII Congreso de Interacción Persona-Ordenador, II Congreso Espanol De Informatica - CEDI 2007)*, 333–342.
- [2] Iwerks, Glenn S., Hanan Samet, and Ken Smith. "Continuous K-Nearest Neighbor Queries for Continuously Moving Points with Updates." *Proceedings 2003 VLDB Conference 29* (August 9, 2003): 512-23. Accessed October 02, 2017. doi:10.1016/b978-012722442-8/50052-5.
- [3] Shan, C., S. Gong, and P. W. McOwan. "Beyond Facial Expressions: Learning Human Emotion from Body Gestures." *Proceedings of the British Machine Vision Conference 2007*, September 2007, 43.1. Accessed October 1, 2017. doi:10.5244/c.21.43.

Modelling Protostellar Disk Formation with C++

Austin Bane

Sponsor: Dr. Fleenor

Roanoke College

Introduction:

The purpose of this project was to produce a modeling software for simulating the transformation of a molecular dust cloud into a protostellar disk. A variety of factors influence the formation of a protostellar disk, but for the purpose of this project we focused on gravity, collision detection, and fluid-particle interactions.

Star formation occurs within molecular clouds of a density that is high relative to the surrounding interstellar medium, but still near vacuum conditions. A cloud is gravitationally bound, meaning the gravitational potential energy, or GPE, is in equilibrium with the other forms of energy, such as thermal energy, which tend to push matter outward. The process of transformation from cloud to protostellar disk and then to protostar occurs when the GPE overwhelms the other forms of energy and the cloud can begin to collapse.

Literature Review:

Vine, one of the top programs used for astrophysical modelling, offers a developed system for general modelling purposes, from galaxy collisions to globular clusters. The assumption made for much of the Vine software is that of a collisionless system, generally achieved through a softening range, wherein if two objects come within some range, they are considered to have merged (Nelson). This assumption makes calculations quicker, allowing for quick calculations of collisions in the space between large numbers of particles.

Simulation:

The program created during this project is called ProtoStarSim. ProtoStarSim takes user input to define a size of the space and a quantity of particles to be generated with certain parameter conditions, such as initial mass, radius, position, and velocity. The position and velocity are randomly generated so that the particles are contained within the space and the velocity is within bounds set by the user. Once the particles have been generated, the user can choose to run a simulation, providing the path to the generated file and a number of timesteps to process. The user can choose to generate a file specifying the current condition of each particle at every timestep or only after the simulation has been run. This allows the user to begin the simulation from any step in the time span or from the end of the time span.

The simulation divides the space using an octree until a user specified base case is reached, either the number of particles in the space or the size of the enclosed space. After the space is divided, the simulation processes gravitational forces on each particle from the neighboring particles in its octant, as well as a center of mass force approximation of each neighboring octant in the parent node. This approximation helps limit the time used for calculation of the gravitational forces while also limiting the error due to approximation. The velocity of each particle is updated from the gravitational forces, after which the program checks for collisions.

The collision algorithm runs with a $O(n^2)$ where n represents the number of particles in a given octant. Particle collisions are checked only within each particles octant, where the particle is compared with all the neighboring particles. Due to the size of the space enclosed in the octant and the speed of the particles, this approximation is fair and the error propagation is limited to only the particles that have a position near the edges of the octant and a velocity

directed out of the octant. The displacement of the particle is considered to be a point, the center of the particle, moving from one position to another, creating a line segment. Extending this segment gives a line, and the lines generated by two particles can be compared for intersection. If a point of intersection is found, the range of time at which each particle is at that point is calculated to determine if the intersection is a collision. Once every collision has been found, the collisions occurring at the earliest time is processed. Since a collision changes the motion of the resulting particle, a new collision could occur, or a collision could be avoided. So the process is repeated, finding all of the collisions and processing each time range until no new collisions are found.

The collision algorithm, while slow, offers a more accurate method for detecting collisions than is often used in astrophysical particle simulation. The algorithm could be further improved by implementing a check for cylinder intersection, since a particle occupies three-dimensional space, so must its displacement create a three-dimensional shape.

Once the gravity and collision portions of the program have been processed, the octree is recreated to account for collided particles and particles that may have moved from one octant to another. The program also removes particles that have escaped the bounds of the space to lower the simulation time.

Results:

The results of the simulation showed high rates of particle escape from the space and low levels of collision. There is no friction slowing the movement of the particles, creating the opportunity for particles to be launched out of the space, and because the particles are often long distances from another, the rate of collisions may be particularly low.

On a simulation with 10^6 particles performing 1000 timesteps ran for approximately 12 hours before stopping without error. ProStarSim has not been parallelized and was only tested on a single computer. Given the approximate time frame for protostellar disk formation, on the order of 10^6 years, a full simulation would take significantly longer. The timestep is initialized as one year, though the user may choose a longer timestep. While a longer timestep would decrease the time, it would increase the error of the simulation.

Future Work:

Improvements to the collision algorithm, such as making the displacement three-dimensional, as well as offering the user more control over the program are the next steps in the process. Additionally, incorporating viscosity between the particles and the surrounding gas and softening the gravitational effect between particles would improve the accuracy of the program.

References:

- Bodenheimer, P. H., "Principles of Star Formation," (2011).
- Schulz, N. S., "The Formation and Early Evolution of Stars," (2012).
- Nelson, A. F., Welzstein, M., Naab, T., Burkert, A., "Vine – A Numerical Code for Simulating Astrophysical Systems Using Particles I: Description of the Physics and the Numerical Methods," The Astrophysical Journal Supplement Series 184, 298-325 (2009).

Term Extraction from Historical Articles using the Stanford Parser

Drew Luther

Advisor: Dr. Anil Shende

Math, Computer Science, and Physics Department

Roanoke College

Problem

One major step in historical research is the literature review. During this step, a researcher looks for secondary papers on the topic to figure out discussions are taking place and find avenues for detailed study.

To assist in this, we use natural language processing and statistical analysis to determine what terms are important for a given topic. This can be used to expand the scope of research or aid in a literature review by providing a quick view of important questions in the document set.

Specifically, we looked at using grammatical information provided by the Stanford Parser to extract terms.

Literature Review

A concise overview of the existing research into term extraction is offered by Heylen and De Hertog [HDH14]. They found that most modern term extraction algorithms use both grammatical/morphological data from Point of Speech taggers and statistical information like how many times term candidates show up in a corpus. This results in a higher accuracy than either method on their own. They also note that a system that works well to extract terms from one corpus might not achieve acceptable results in a corpus from a different field.

Although systems exist for fields like medicine, the features for term extraction are significantly different. Most medical terms will be proper nouns, but many historical terms are multi-word terms that are constructed from common nouns and modifying words like adjectives.

The Stanford Parser is a natural language processing tool developed by the Stanford University Natural Language Processing Group [NdMG+ 16]. It takes plain text as an input and stochastically determines the grammatical structure of the input as shown in Figure 1.

Term Extraction

After running the Stanford Parser on the plaintext, our program parses through the output and constructs a list of terms. The terms are either words tagged by the Parser as NNP/NNPS (proper noun) or the contents of a noun phrase (tagged NP). Articles (tagged DT) are ignored to avoid listing the same term twice. For example, the terms extracted from Figure 1 would be “Kentucky”, “early beachhead”, “bluegrass district”, and “slavery”.


```

(ROOT
(S
  (PP (IN In)
    (NP (NNP Kentucky)))
  (, ,)
  (NP
    (NP (DT an) (JJ early) (` `) (NN beachhead) (' '))
    (PP (IN in)
      (NP (DT the) (JJ bluegrass) (NN district))))
  (VP (VBD allowed)
    (S
      (NP (NN slavery))
      (VP (TO to)
        (VP (VB become)
          (ADJP (RB firmly) (JJ entrenched))
          (, ,)

```

Figure 1: Output from Stanford Parser

For the extraction of terms, only one NP is used for each term. The Parser can tag parts of an NP as a subordinate NP, which would result in many terms that were made up of actual terms. By limiting a term to a single NP instead of multiple levels, some terms are misread as two separate terms which decreases the accuracy of the term extraction, but it is fairly common for a large chunk of a sentence to be tagged as an overarching NP so the overall accuracy is increased.

Results

Our program finds most meaningful terms in test documents. Although it currently includes phrases that aren't terms or are missing context, the frequency of occurrence for terms is tracked which allows for a simple check for the validity of a given term. Terms that show up more frequently are more likely to be meaningful.

Future Work

Future work includes improving the term extraction through frequency analysis and other statistical techniques as well as calculating conditional probability of a term showing up in the same sentence as another term to show relations between the two. Later work will include the automatic discovery of historical articles from online databases and websites for easy public use.

References

[HDH14] Kris Heylen and Dirk De Hertog. Automatic term extraction. *Handbook of Terminology*, 1:199-219, 2014.

[NdMG+ 16] Joakim Nivre, Marie-Catherine de Marneffe, Filip Ginter, Yoav Goldberg, Jan Hajič, Christopher D. Manning, Ryan McDonald, Slav Petrov, Sampo Pyysalo, Natalia Silveira, Reut Tsarfaty, and Daniel Zeman. Universal dependencies v1: A multilingual treebank collection. *LREC 2016*. LREC, 2016.

Visualizing Molecules Using Augmented Reality and Image Recognition

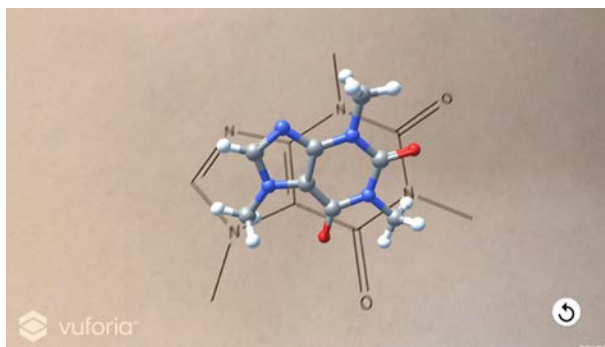
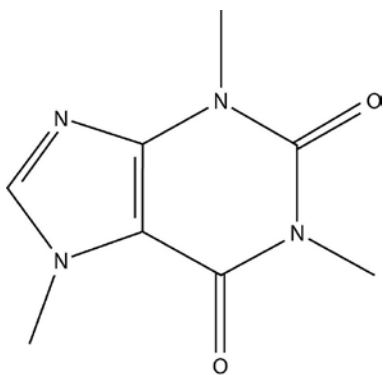
Mike Deiters and Kevin Stevens

Georgia Gwinnett College

Faculty Sponsors: Dr. Derek Behmke and Dr. David Kerven

Augmented reality provides an extra layer of information over the user's view, typically through the use of a camera lens and a screen. Using augmented reality, end users are able to see more information about the world around them, such as the store or restaurant they are currently looking at. When used in conjunction with image recognition, a device can recognize symbols, pictures, and letters; for instance, it may recognize a sign on the street and translate it to the user's native language. These technologies can give users insight into the world around them and help visualize it in new ways that would otherwise be impossible.

Chemistry students learn about microscopic molecules that are usually represented as 2D diagrams on paper, but if they want to view them as the 3D structures that they actually are, they have to use a molecular modeling kit. This kit contains many small parts which the user may snap together to construct a molecule, but can be extremely inconvenient for numerous reasons. It takes up room in their bag, the number of pieces they carry limits which and how many molecules they can make, it's time consuming to construct the molecules, and as with anything that comes with many small parts, it's likely that many kits will be incomplete by the second month of the semester. Due to these inconveniences, an app which would let students use their phone or tablet to view a 3D model of a molecule using augmented reality and image recognition could be very useful.



Caffeine as represented by a traditional 2D model and by a 3D model in our app.

Early in the technology's life, educators realized that augmented reality could be a useful tool for teaching. A medical student could use it to effectively see inside their subject while practicing surgery; a technician could use it to see inside a device and learn its parts [1]; an astronomy student could use it to interact with a 3D representation of the solar system [4].

However, back then, one needed an expensive head-mounted display to take advantage of it, greatly limiting its accessibility. However, consumer devices have caught up, and today, students have access to smartphones and tablets whose camera and screen allow them to take advantage of augmented reality. Although this isn't quite as immersive as a head-mounted display, a study has still shown that interacting with a molecule through the tactile interface of a touch screen can improve the user's learning ability over traditional 2D images [3].

Vuforia is a tool for augmented reality and image recognition. Its Target Manager allows us to set up a database that links image targets to display objects. Vuforia extracts features from the image targets and stores them in a database that can be downloaded and packaged within an application [2]. When the application is running, the image recognition software analyzes the view through the device's camera, and if it sees an image that matches a target in its database, retrieves the appropriate data. This may be a pre-built 3D model, or data that allows models to be created dynamically. For our purposes, we retrieve the molecules from the PubChem database [5] as mol files, which define the molecule's atoms and structural bonds. Using this information, we're able to construct the molecules as 3D objects for the user to view and interact with through augmented reality.

Using augmented reality and image recognition together, we've created an application for smartphones and tablets which allows the user to use the device's camera and a picture of a molecule to view that molecule in three-dimensional space, which they may interact with and view from any angle as if it actually exists in the real world. With this application, chemistry students will be able to easily view molecules as 3D models that are more accurate and easier to understand than limited 2D drawings, but without needing to carry around a molecular model kit.

References:

- [1] Billinghamurst, Mark. "Augmented reality in education." *New Horizons for Learning* 12 (2002).
- [2] Image Targets, Vuforia,
<http://library.vuforia.com/content/vuforia-library/en/articles/Training/Image-Target-Guide.html>. Accessed 26 Sept. 2017.
- [3] McCollum, Brett M. "The Effects of Using Touch-Screen Devices on Students' Molecular Visualization and Representational Competence Skills." *Journal of Chemical Education* 91 (2014).
- [4] Shelton, B. "Augmented Reality and Education." *New Horizons for Learning* 9.1 (2002).
- [5] The PubChem Project. <https://pubchem.ncbi.nlm.nih.gov/>. Accessed 01 October 2017,
Contributors: Dr. Julia Paredes and Dr. Richard Pennington

MR. Mol: Mixed Reality Molecule

GEORGIA GWINNETT COLLEGE

AUTHORS | Robert “Jory” Alexander, Matthew Camp, Pedro Garcia, Anastasiya Golovan, Jacob Piazza, GinaAnn Rosbury
ADVISORS | Dr. Evelyn Brannock and Dr. Robert Lutz

INTRODUCTION AND PURPOSE

Our research group, inspired by an augmented reality (AR) experiment created by the Georgia Gwinnett College (GGC) Chemistry Department, has partnered with GGC faculty in an interdisciplinary effort to create an application that allows the user to manipulate and simultaneously compare molecules projected by the Microsoft HoloLens, a mixed reality (MR) device. Our program builds on and improves an initial AR effort that combined smartphones, tablets, and Aurasma to convert a 2D molecule structure drawn on paper into a 3D object, enabling the user to interact with the molecule on their device (1). While the initial experiment allows for active learning, there are restrictions such as having to hold the device over the 2D drawing to view the 3D molecules in Aurasma. Viewing capacity is also limited to the size of the device screen. Instead of pursuing an AR learning environment, our team has decided to take it a step further and provide a fully interactive MR learning experience for the user via the Microsoft HoloLens headset.

Our team is pursuing the simulation of a kinesthetic learning experience for studying molecules in the classroom. MR brings a sense of realness to an otherwise impalpable object. Students can have a simulated hands-on learning experience with objects that are typically limited to 2D. The 3D nature of molecular structures has a dramatic impact on their chemical and physical properties. Many molecular structures have complex characteristics that are lost when represented in a 2D form. When students are unable to visualize the 2D representations of molecules in 3D, they struggle to understand molecular properties and concepts such as stereochemistry. MR fortifies learning by removing the constraints of working with a flat projection and offers an engaging platform to challenge how students and educators alike interact with molecular visualizations (2). In our case, users can omni-directionally study a molecule and even compare molecules, allowing for a deeper comprehension and understanding of the molecules' physical composition and chemical interactions. The holographic model has differentiating advantages over tactile learning tools, like plastic molecular model kits, because molecular structures can be preloaded and do not have to be put together manually. The ability to scale gives users various accurate perspectives and details of particularly complex structures.

PROOF OF CONCEPT

The proof of concept is a prototype application that allows for the manipulation of molecules projected by the Microsoft HoloLens. The custom HoloLens application displays molecular structures in a mixed reality environment, allowing the user to maneuver (select, move, scale, and rotate) and compare two molecules simultaneously. The user can even “walk around” the molecule if they desire while combining gaze, voice and gesture commands.

HARDWARE AND SOFTWARE IMPLEMENTATION

Mixed reality (MR) is a blend of the real world and the virtual world in which physical and digital objects exist and interact in real time. With the rise of interactive technology, many acquisition devices have been introduced which allow the user to control the device without touching the keyboard, the mouse, or the screen (3). Devices like the Microsoft HoloLens “break down the barriers between virtual and physical reality,

and enable the physical and virtual worlds to intersect in new ways” (4). Instead of either being completely cut off from the outside world, as with virtual reality (VR), or being confined to viewing a 3D object on a screen, as with augmented reality (AR), MR provides an immersive experience that merges holograms into the user’s physical environment while allowing the high-quality holographs to be viewed from all directions (2, 4). The HoloLens is a self-contained system that generates and projects stereographic images onto the lenses of a headset (4). In addition to having a central processing unit, the HoloLens contains a separate holographic processing unit that allows 3D graphics to exist in the user's physical space while keeping track of user input such as voice commands and gestures (4). Because the HoloLens uses tracking that combines data from multiple input sensors and cameras with algorithms, the device is able render a smooth MR experience (5).

We are implementing the use of the Microsoft HoloLens and the Unity Game Development Engine in order to develop directly into the HoloLens. Our program allows a user to select two molecules to examine and compare as needed from a list. Once selected, the molecule is displayed. Molecule data is retrieved from the PubChem website (6) and procedurally built as a hologram. Using a combination of gaze, voice, and gesture controls, users can select, reposition, rotate, scale, and reset the molecular structures, via selecting from the menu or via voice command, to get a better understanding of their characteristics. Figure 1 to the right shows a snapshot of our application’s user interface.



Figure 1

CONCLUSION

Mixed reality (MR) creates an immersive environment with virtual objects inlaid into the real world. This interactive setting is optimal for exploring the intricate 3D characteristics of molecular structures. The use of gaze, voice, and gesture controls allow for easy manipulation of the holographic molecules. Combined, these features enhance both teaching and learning by bringing otherwise 2D objects to life.

REFERENCES

1. Pennington, Richard, Behmke, Derek & Lutz, Robert (2016, 24 August). *Aurasma / Chem* [Video file]. Retrieved from media.ggc.edu/media/t/1_u83n4h8a
2. Hoffman, M., & Provance, J. (2017). Visualization of molecular structures using HoloLens-based augmented reality. *AMIA Summits on Translational Science Proceedings, 2017*, 68–74.
3. Tran, V., Lee, J., Kim, D., & Jeong, Y. (2016). Easy-to-use virtual brick manipulation techniques using hand gestures. *Journal of Supercomputing*, 72(7), 2752. doi:10.1007/s11227-015-1588-4
4. Noor, A. K. (2016). The HoloLens Revolution. *Mechanical Engineering*, 138(10), 30-35.
5. Marvin, R. (2017). Microsoft’s Mixed-Reality Plans Go Far Beyond HoloLens. *PC Magazine*, 111-116.
6. https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST.html and <https://pubchem.ncbi.nlm.nih.gov>, retrieved on 10/1/2017. Retrieved on 10/1/2017.

Special acknowledgement and thanks to **Dr. Derek Behmke**, *Assistant Professor of Chemistry*, **Dr. Julia E. Barker Paredes**, *Associate Professor of Chemistry*, **Dr. Richard Pennington**, *Associate Professor of Chemistry* and **Dr. David Kerven**, *Associate Professor of Information Technology* at *Georgia Gwinnett College* for their significant time and contributions.