ABSTRACT

Molecular scientists have made quite a progress to engineer Nano-scale molecular structure, engineering molecular dynamics (MD) and flexibility is a new challenge every day. Dynamics at the molecular scale differs from the familiar mechanics of everyday objects because it involves a complicated, highly correlated, and three-dimensional many-body dynamical choreography which is often non-intuitive even for highly trained researchers. We recently described how interactive molecular dynamics in AR can help to meet this challenge, enabling researchers to manipulate real-time MD simulations of flexible structures in 3D.

INTRODUCTION

Inspiration

Complex protein structures in scientific journals can be a challenge to understand since it is hard for a student or an expert to visualize complex 3D molecular structures.

We want to build something on the new ARKit that's both useful and fun to make. In 1977, artificial and augmented reality pioneer Myron Krueger began his paper Responsive Environments with the observation that “human-machine interaction is usually limited to a seated [person] poking at a machine with [their] fingers or perhaps waving hands over a data tablet.”. Krueger went on to speculate that real-time, multi-sensory interaction between humans and machines might enable exciting and efficient new approaches for exploring realities that are otherwise impossible to access. Nanoscale molecular objects offer fertile testbeds for exploring new technological frontiers in human-computer interaction (HCI), owing to the fact that molecules represent objects that are important to society and industry, but which we are unable to directly perceive, and which are characterized by considerable three-dimensional dynamic complexity.

As Krueger observed, the sensory modes we use to obtain insight and navigate the complex and dynamic terra incognita of nanoscale structures are limited: our representational methods are confined mostly to 2d, and primarily designed for parsing by our visual cortex (plots, images, movies, articles, etc.). Recent research in psychology and neuroscience has shown that our attention is enhanced when we engage in multi-sensory processing, 2, 3 simultaneously integrating complex data across our various sensory channels, spanning the visual, auditory, olfactory, and somatosensory cortexes. In some sense, we do not make full use of the array of sensory, perceptual, and information processing machinery which we have evolved as thinking and feeling beings to make sense of the natural world around us. This not only limits our ability to understand the 3D complexity of dynamical microscopic systems; in many cases it is also extremely inefficient. Beyond a relatively small size threshold of ~50 atoms, 2D representational tools quickly become unwieldy for handling 3D molecular systems. For example, researchers lose lots of time struggling with 2D molecular viewers to build complex 3d structures, attempting to represent 3D structural dynamics in a 2D presentation format, or fighting with

scripting languages to undertake complex 3D molecular manipulations. Over the past several years, various laboratories have been carrying out an interdisciplinary research program exploring interactive molecular dynamics (iMD) beyond standard 2D interfaces, designed to enable direct multisensory interaction with molecular simulations. The recent emergence of robust and affordable augmented reality (AR) technologies has been a key enabler in these efforts, allowing us to develop a framework where scientists can manipulate rigorous real-time simulations of molecular systems.

OBJECTIVES

The app uses a smartphone's camera. A user can point to a scientific journal or college textbook. The App parses through the text, extracts chemical compounds and presents a list. A user can choose the molecule/protein he wants to render in the AR environment. The complex 3D structures are then presented which the user can interact physically.

Application includes

1. TextCapture module:

- For previewing the camera layer for text recognition, we make use of AVCaptureSession.
- We perform text recognition using ABBY Real-Time Recognition SDK.
- On recognition of stable text input from camera & ABBYY SDK, locally it is processed for an API request.
- API call for fetching list of chemical elements/molecules/proteins are obtained by Wit.AI backend which helps in mapping local DAE models for ARView.
- On selected chemical to view in AR, the AR module is initialized for rendering the local DAE model to display on ARView.

2. AR Module:

- For rendering the AR model, we initialize ARSCNView with ARWorldTrackingConfiguration, for the chosen chemical.
- renderScene() render's with geometrical orientation & rotation of the AR model which is mapped for chemical (DAE chemical model present locally in the asset).
- Using SCNText to display along with the AR model in a scene the additional information of the chemical compound such as average mass, molecular weight, molecular formula, and common name.

Chemical AR Model flask service includes

PyMOL- PyMOL is an open-source molecular visualization system created by Warren Lyford DeLano. It was commercialized initially by DeLano Scientific LLC, which was a private software company dedicated to creating useful tools that become universally accessible to scientific and educational communities. It is currently commercialized by Schrödinger, Inc. PyMOL can produce high-quality 3D images of small molecules and biological macromolecules, such as proteins. According to the original author, by 2009, almost a quarter of all published images of 3D protein structures in the scientific literature were made using PyMOL.
PyMOL is one of a few open-source model visualization tools available for use in structural biology. The *Py* part of the software's name refers to the program having been written in the programming language Python.
PyMOL uses OpenGL Extension Wrangler Library (GLEW) and FreeGLUT and can solve Poisson–Boltzmann equations using the Adaptive Poisson Boltzmann Solver.[2] PyMOL used Tk for the GUI widgets and had native Aqua binaries for macOS through Schrödinger, which were replaced with a PyQt user interface on all platforms with the release of version 2.0.

AbbyyRtrSDK- A premium mobile onboarding process offers your customers a frictionless way to capture and provide a self-servicing trailing document to increase retention rates. Power your app with Mobile Capture and deliver exceptional customer experiences by making mobile document capture easy for your customers with a simple process: point and capture. ABBYY Mobile Capture is an SDK that offers automatic data capture within your mobile app, providing real-time recognition and capturing photos of documents for on-device or back-end processing.

OpenGL- OpenGL is the premier environment for developing portable, interactive 2D and 3D graphics applications. Since its introduction in 1992, OpenGL has become the industry's most widely used and supported 2D and 3D graphics application programming interface (API), bringing thousands of applications to a wide variety of computer platforms. OpenGL fosters innovation and speeds application development by incorporating a broad set of rendering, texture mapping, special effects, and other powerful visualization functions. Developers can leverage the power of OpenGL across all popular desktop and workstation platforms, ensuring wide application deployment.

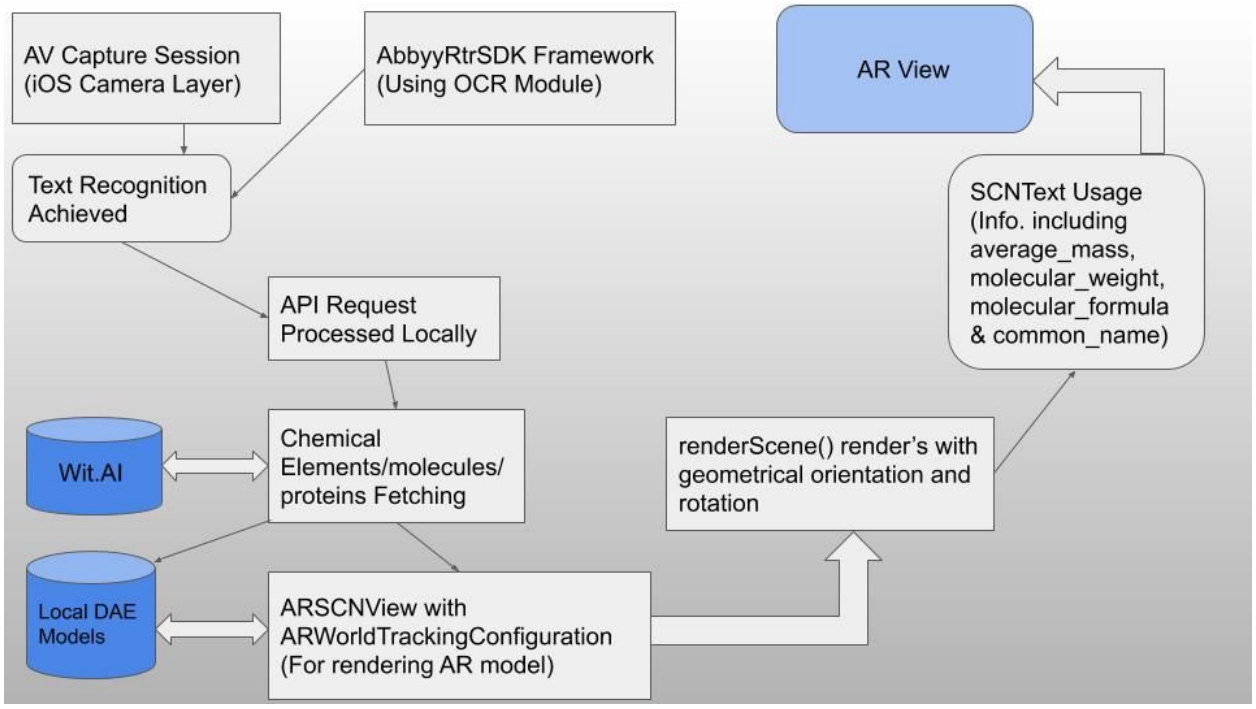
MeshTool- This is a super powerful tool that can make your vector illustrations look more 3D, or photorealistic. It works by adding a 'mesh' over a closed shape, the lines of the mesh intersecting at points onto which different color swatches can be applied to create a vectorized image.

ChemSpider- *ChemSpider* is a free chemical structure database providing fast text and structure search access to over 67 million structures from hundreds of data sources.

PROPOSED SYSTEM

We intend to build a complete AR-based application to determine the molecular integrity of a chemical compound. The application can capture the text of the chemical compound using a phone's camera, creating an augmented reality on the camera space to display a 3D chemical compound.

SYSTEM ARCHITECTURE



SYSTEM REQUIREMENTS

- Mac System
- Mac OS X Version 10+
- Intel Core i5 or above.
- 4 GB Memory
- Xcode
- IPhone
- Apple Developer Account

METHODOLOGY

How we build-

The App extracts chemical names from a large text in real-time and renders the molecules/proteins in an AR environment.

- Get real-time text from the camera.
- Find Chemical compounds/molecules/proteins from the text.
    - Locally pre-trained CoreML model (Chemical named entities recognition model) and AbbyyRtrSDK.
    - Wit.AI for processing keywords/traits and extracting entities
- Fetch the chemical name and search for information on ChemSpider
- The backend service takes a .MOL file containing the molecular data and renders into a 3D scene with OpenGL+PyMOL+MeshTool.
- The rendered .DAE (Collada) files are used to project Chemical formulae as an AR Scene.

INNOVATION AND CONTRIBUTION TO THE FIELD

Challenges we will run into

We have to find a way to automate the .MOL to .DAE conversion. There's no direct way to do it. MOL is a Chemical table file with structure information and .DAE is a 3D scene. The conversion could be done with pyMOL scripts along with a Script automating the whole process.

Accomplishments

Since this is our first AR project. We'd be learning more about CoreML and ARToolKit.

FUTURE SCOPE

- Better MOL rendering, more interactiveness on the 3D scene and better UX. We have plans to port it on to Oculus as well.
- It can be extended to not only show chemical compounds but also reactions between multiple compounds in real-time.
- It can further be improved to perform new reactions that are not in the dataset.
- Can use machine learning techniques to provide suggestions for new chemical bonding with a probable chemical structure based on requirements.

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