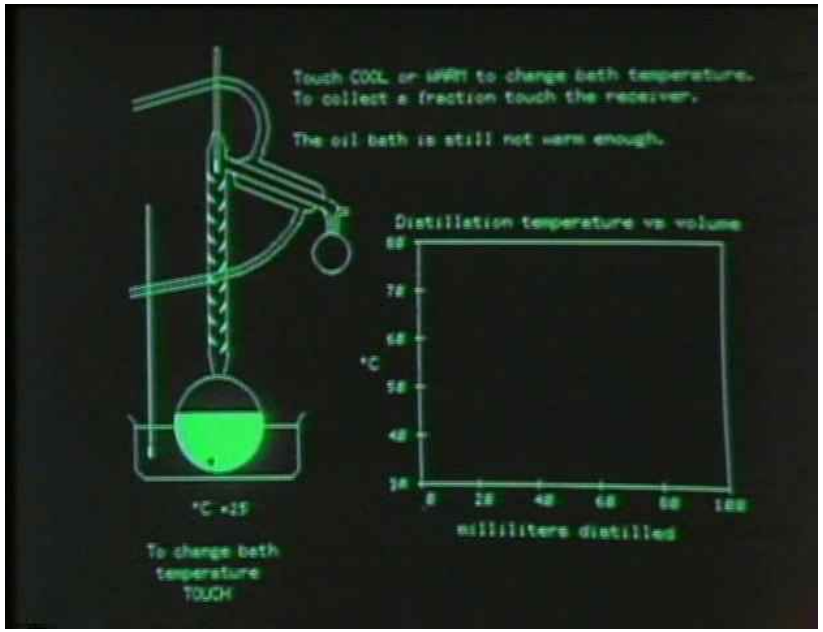
Computer Graphics for Cheminformatics

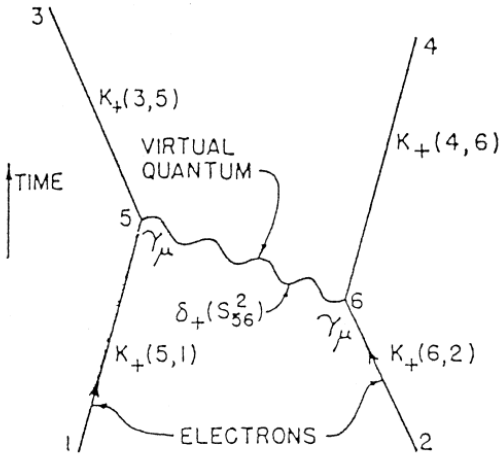
Daniel Probst, University of Bern

Daniel Probst (Me)

1970s and earlier

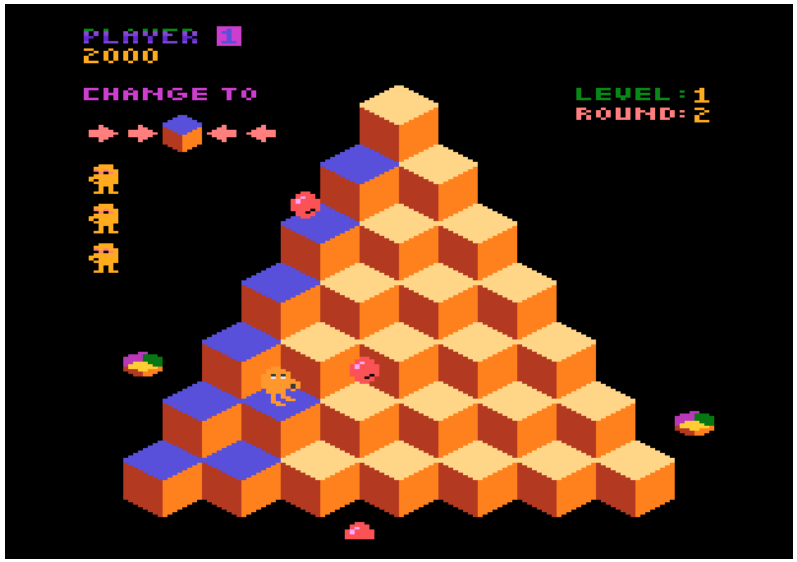


PLATO (Programmed Logic for Automatic Teaching Operations) was the first generalized computer-assisted instruction system.



Feynman, Richard P. "Simulating physics with computers." *International journal of theoretical physics* 21.6 (1982): 467-488.

1980s



Q*bert is an arcade game developed and published by Gottlieb in 1982

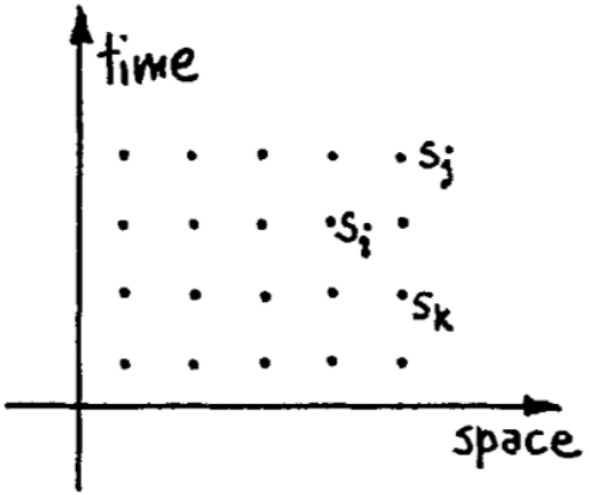


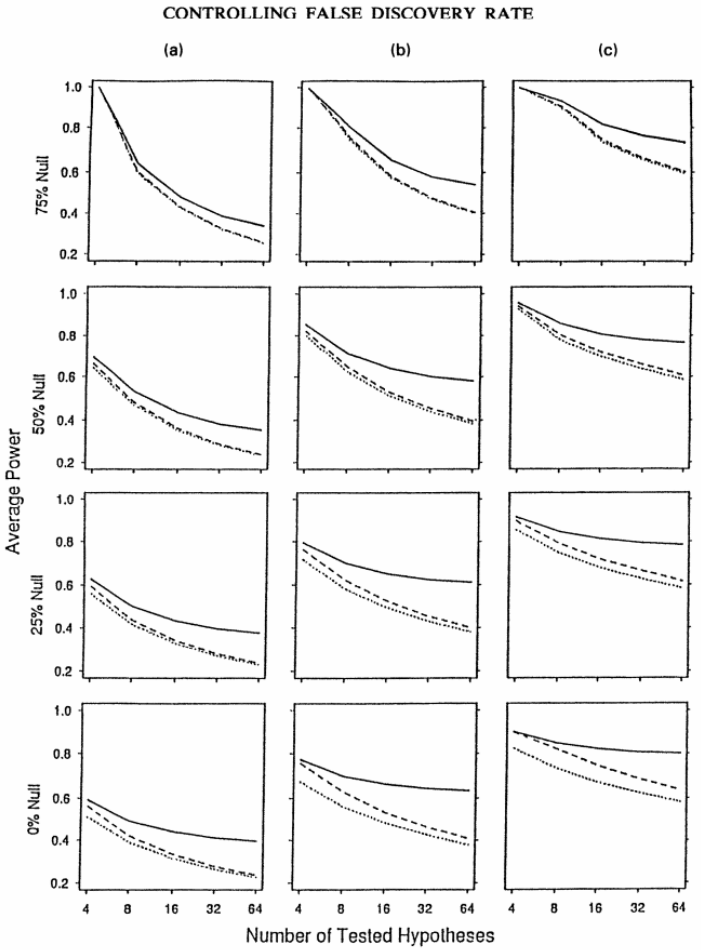
Fig. 1.

Feynman, Richard P. "Simulating physics with computers." *International journal of theoretical physics* 21.6 (1982): 467-488.

1990s

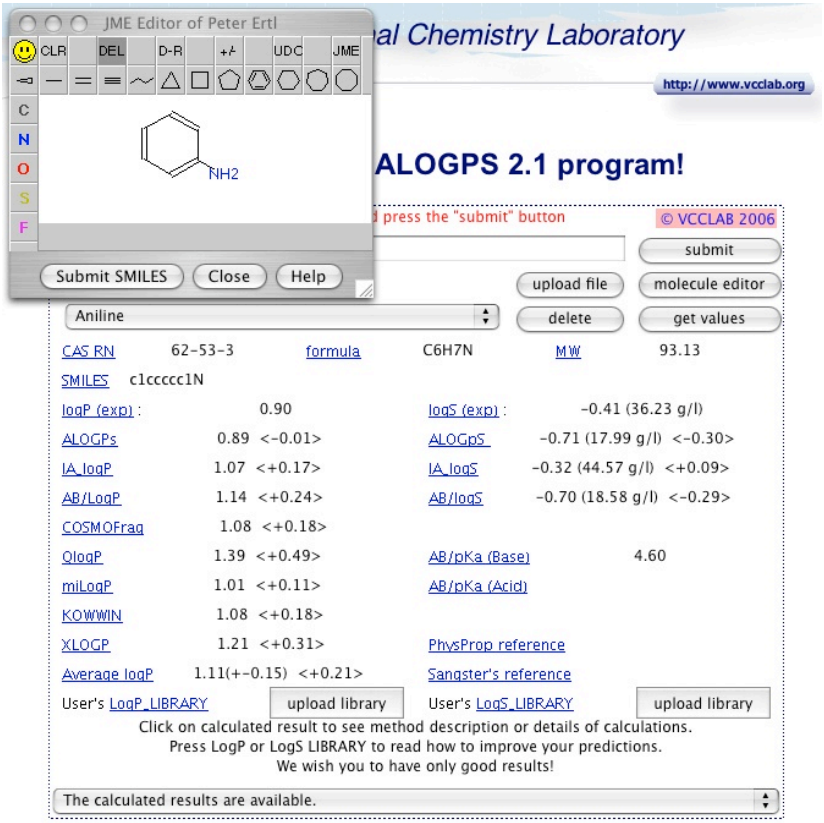
Warcraft II: Tides of Darkness published by Blizzard Entertainment and first released for DOS in 1995

Star Wars: TIE Fighter is a 1994 space flight simulator released by LucasArts



Benjamini, Yoav, and Yosef Hochberg. "Controlling the false discovery rate: a practical and powerful approach to multiple testing." Journal of the royal statistical society. Series B (Methodological) (1995): 289-300.

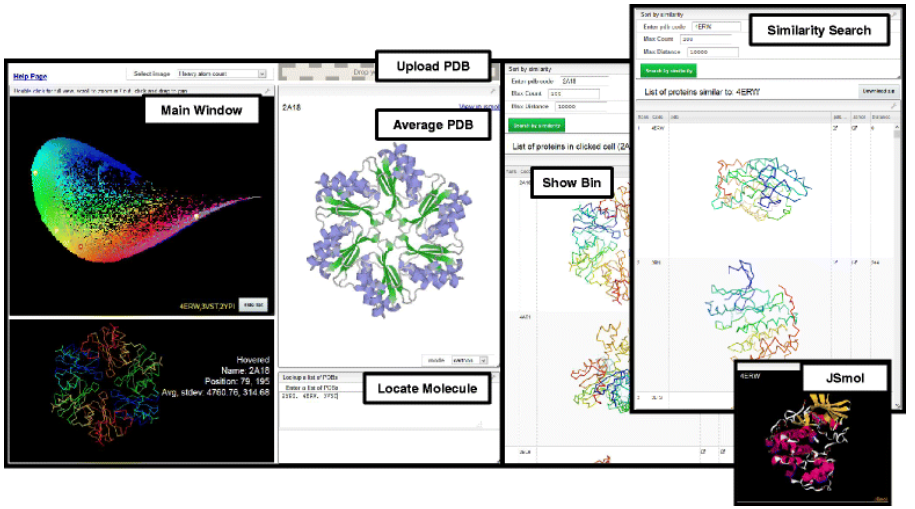
2000s



Civilization IV was designed by Soren Johnson under the direction of Sid Meier and Firaxis Games.
Battlefield 2 developed by Digital Illusions CE

Tetko, Igor V., et al. "Virtual computational chemistry laboratory–design and description." Journal of computer-aided molecular design 19.6 (2005): 453-463.

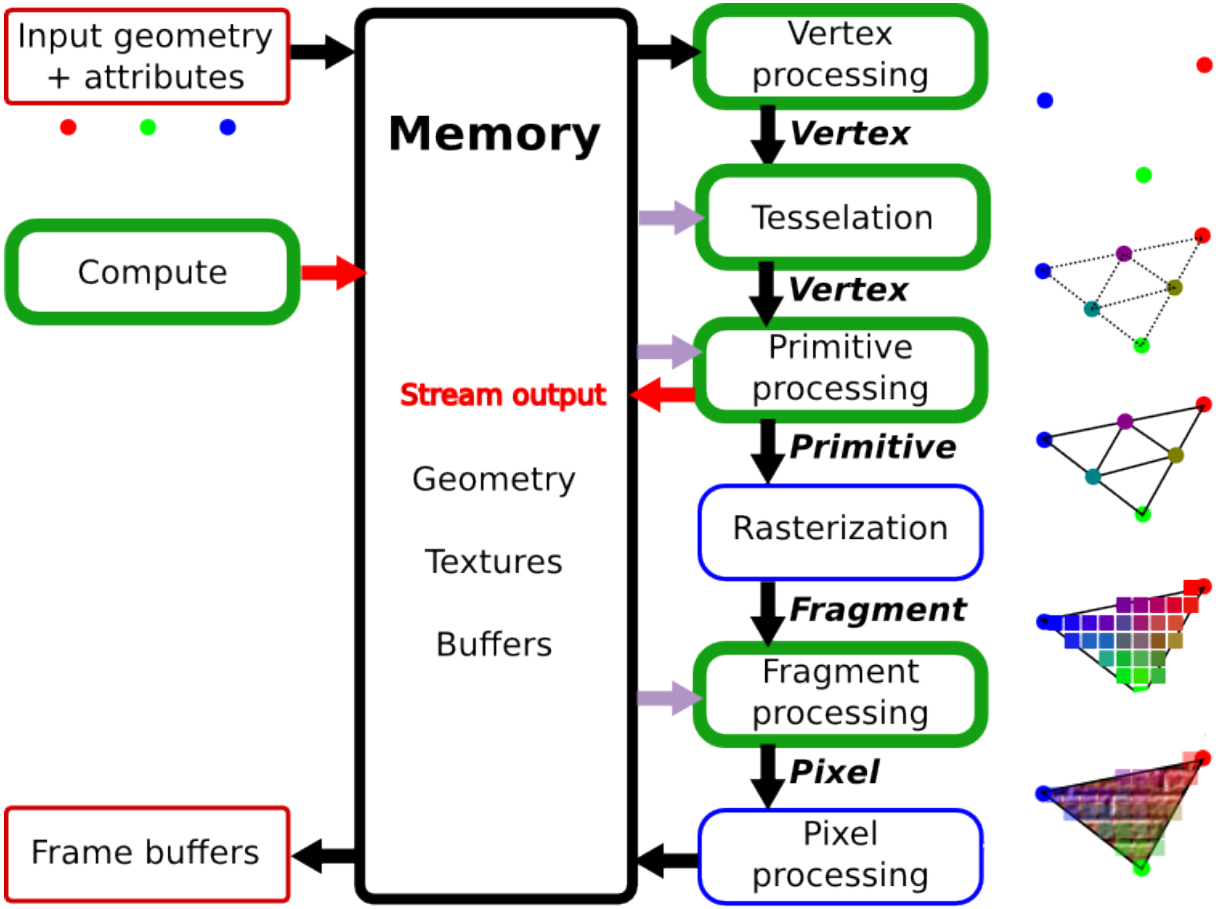
2010s



The Witcher 3: Wild Hunt[a] developed and published by CD Projekt.
Fallout Shelter developed by Bethesda Game Studios

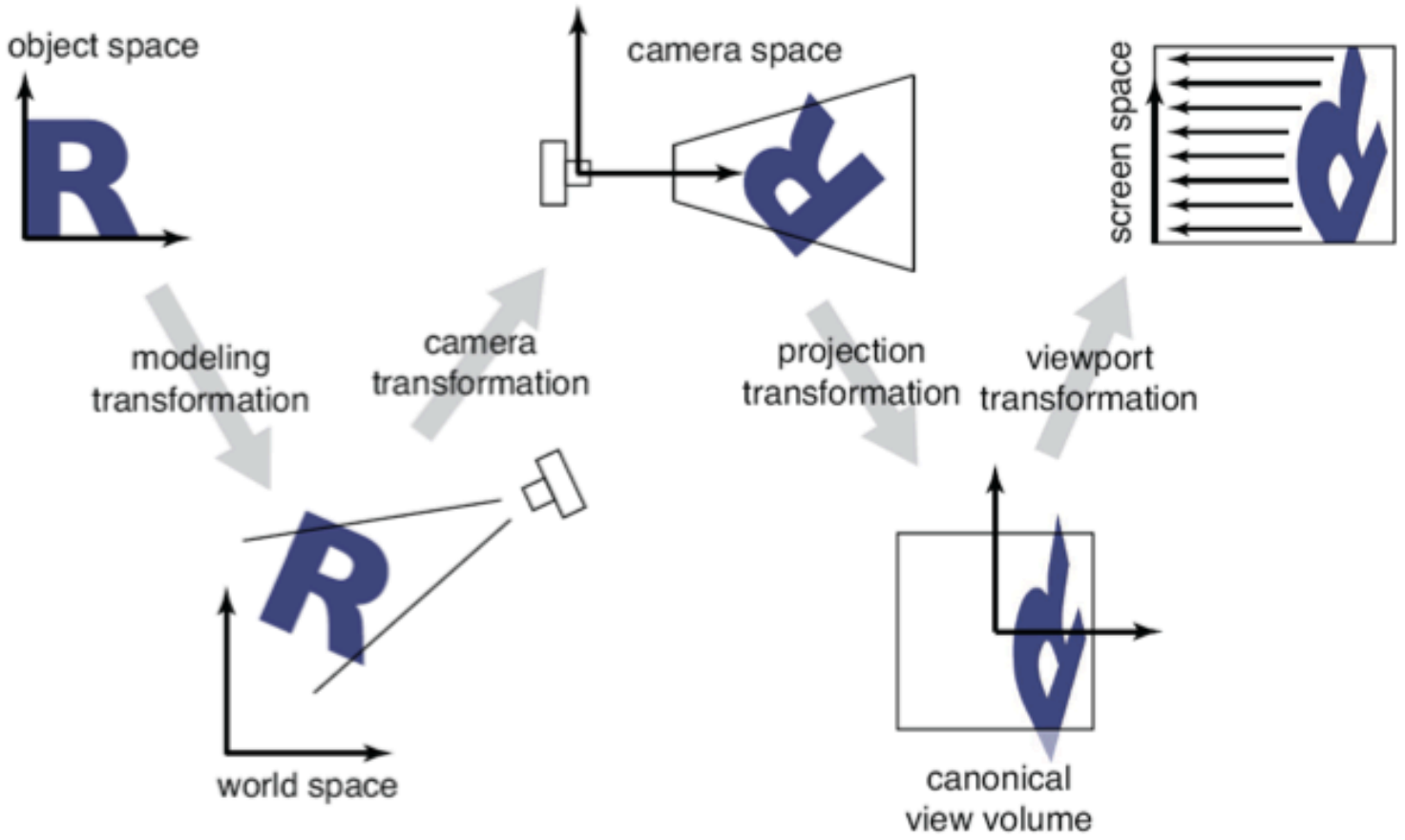
PDB-Explorer: a Web-Based Interactive Map of the Protein Data Bank in Shape Space. X Jin, M Awale, M Zasso, D Kostro, L Patiny, JL Reymond, BMC Bioinform., 2015, 16, 33

Computer Graphics



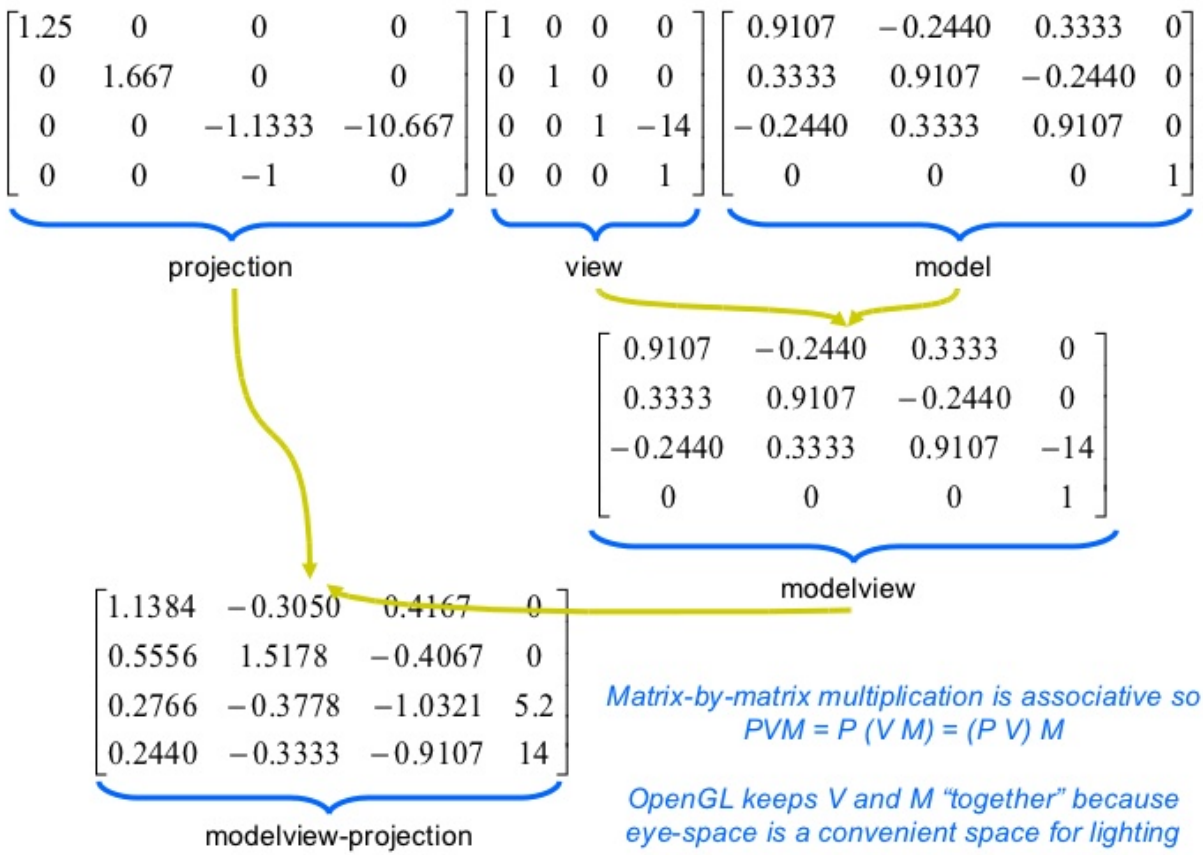
https://github.com/Craigson/Intro_to_shaders

Linear Algebra is Fun

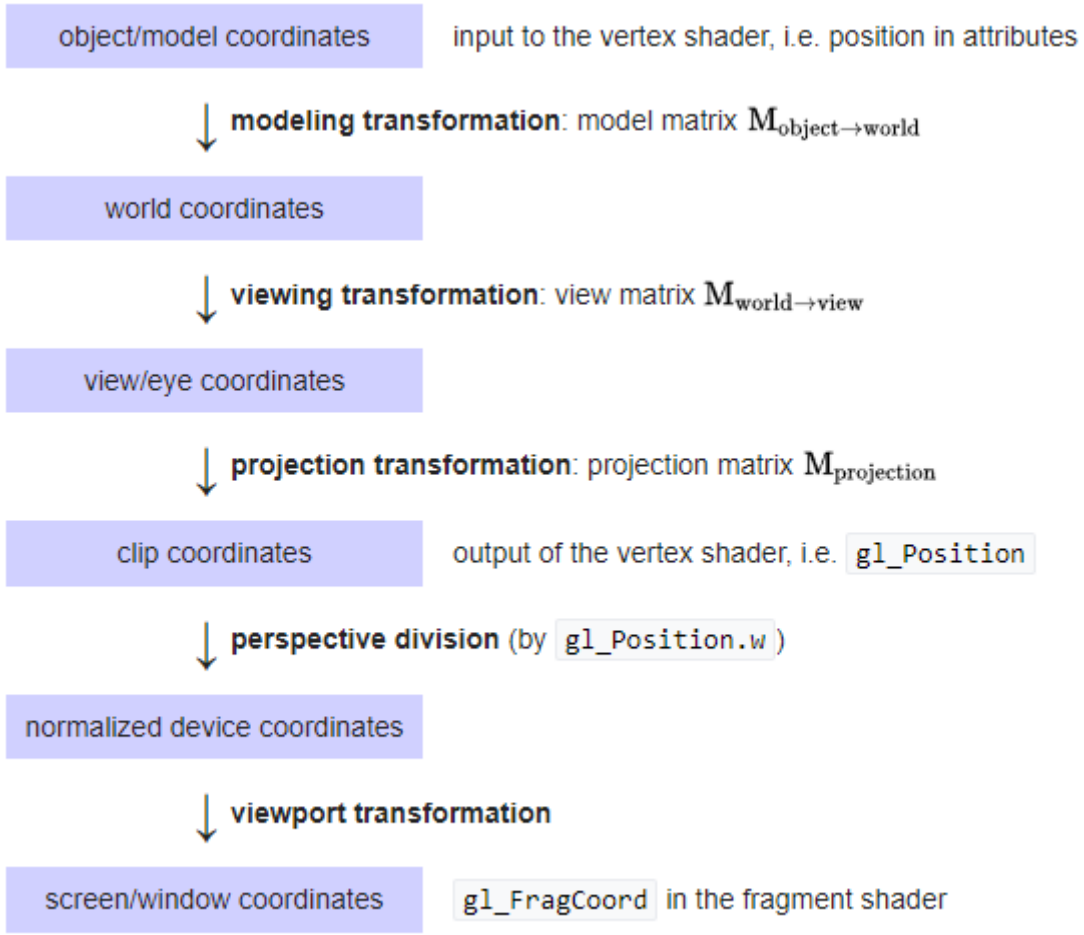


Some guy from a forum

Linear Algebra is Fun

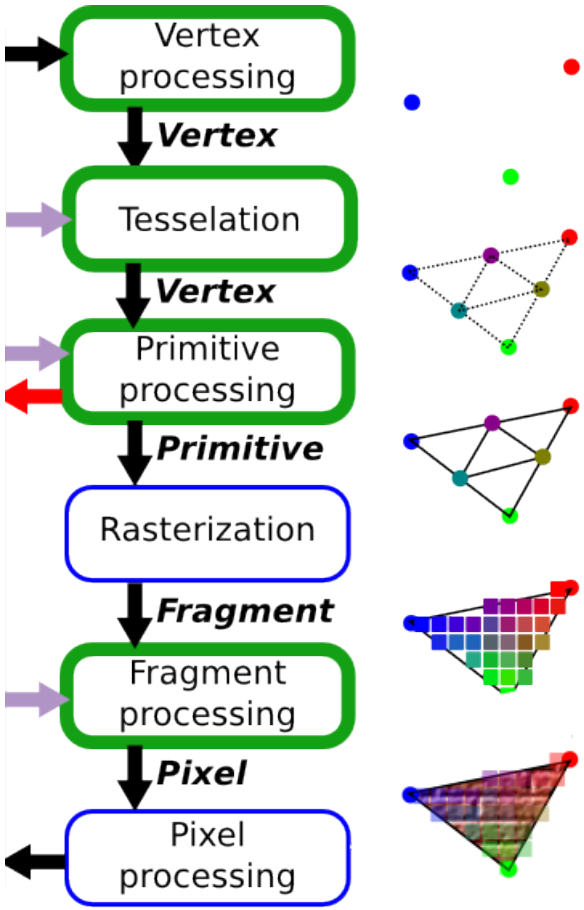


Linear Algebra is Fun



https://en.wikibooks.org/wiki/GLSL_Programming

Shaders



https://github.com/Craigson/Intro_to_shaders

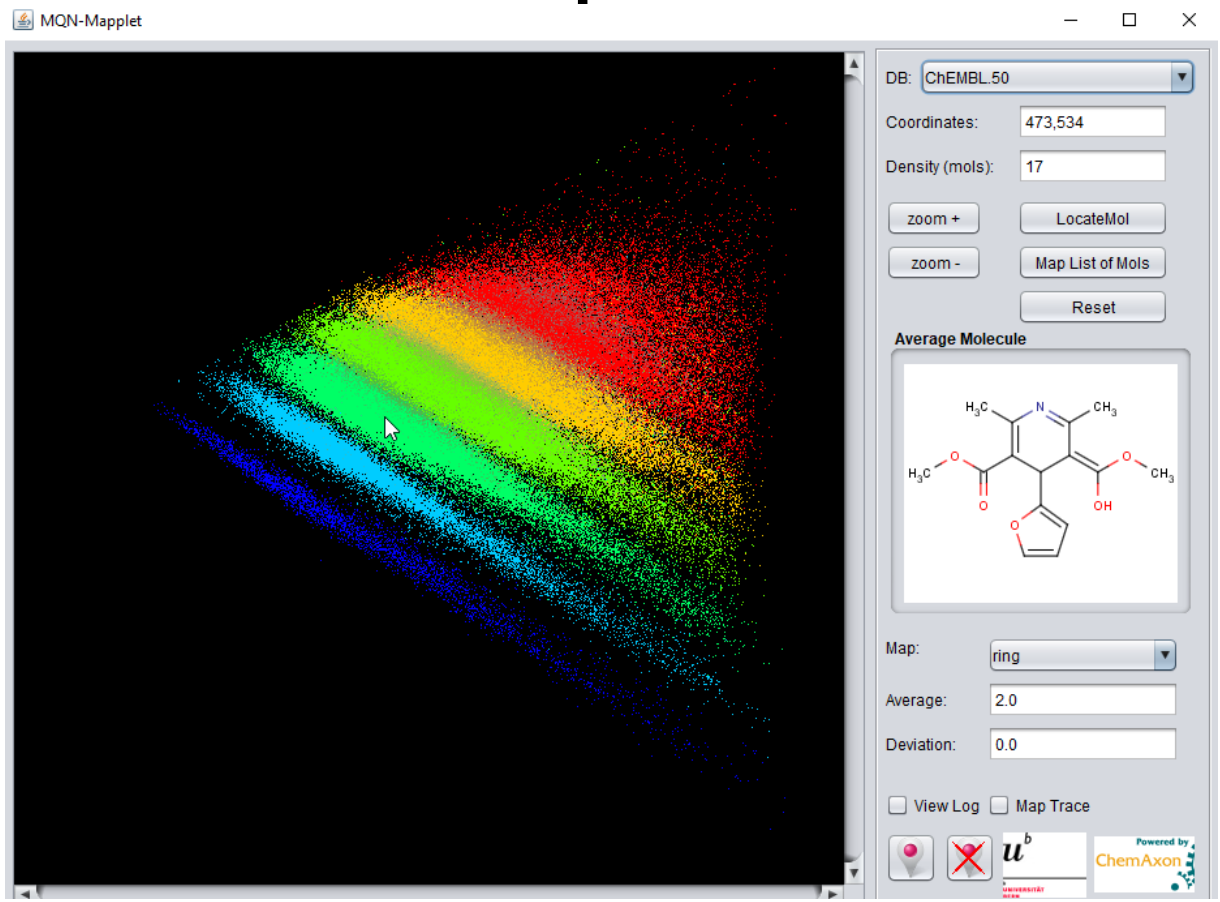
Someone on the Internet

Get Hacking

```
1  #version 150
2
3  in vec4 position;
4  uniform mat4 Model;
5  uniform mat4 View;
6  uniform mat4 Projection;
7
8  void main() {
9    gl_Position = Projection * View * Model * position;
10 }
```

https://shaderfrog.com

Chemical Space



The MQN-Mapplet: Visualization of Chemical Space with Interactive Maps of DrugBank, ChEMBL, PubChem, GDB-11 and GDB-13. M. Awale, R. van Deursen, J.-L. Reymond, J. Chem. Inf. Model. 2013, 53, 509-518.

JavaApplets

Oracle signals the end of Java applet support for browsers

Oracle will depreciate the Java browser plug-in in JDK 9

How to use Java in Google Chrome | Tech Help KB
https://techhelpkb.com/how-to-use-java-in-google-chrome/
Apr 8, 2016 - Learn how to use **Java** in Google **Chrome**, along with other NPAPI plugins like Silverlight and Unity. There is no reason to switch web browsers.

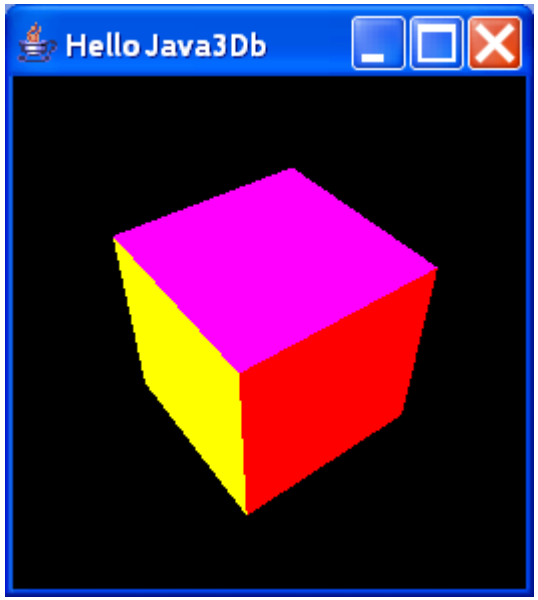
How to enable Java in Google Chrome 42 and higher | THKB
https://techhelpkb.com/enable-java-in-google-chrome-42/
Apr 14, 2015 - Did you start seeing This plug-in is not supported after upgrading **Chrome**? You, and everyone else who uses **Chrome** to view **Java** content in their web browser. When Google released **Chrome** 42, it disabled some historically problematic browser plug-ins by default. Plug-ins, such as **Java** from Oracle and ...

FIX: How To Enable Java In Google Chrome In 2017 - YouTube
https://www.youtube.com/watch?v=QXb8nvpGBIA
Sep 13, 2015 - Uploaded by MDTechVideos
UPDATE: This tutorial still works in 2017. Will only work on **Chrome** installations on Windows machines. Mac ...

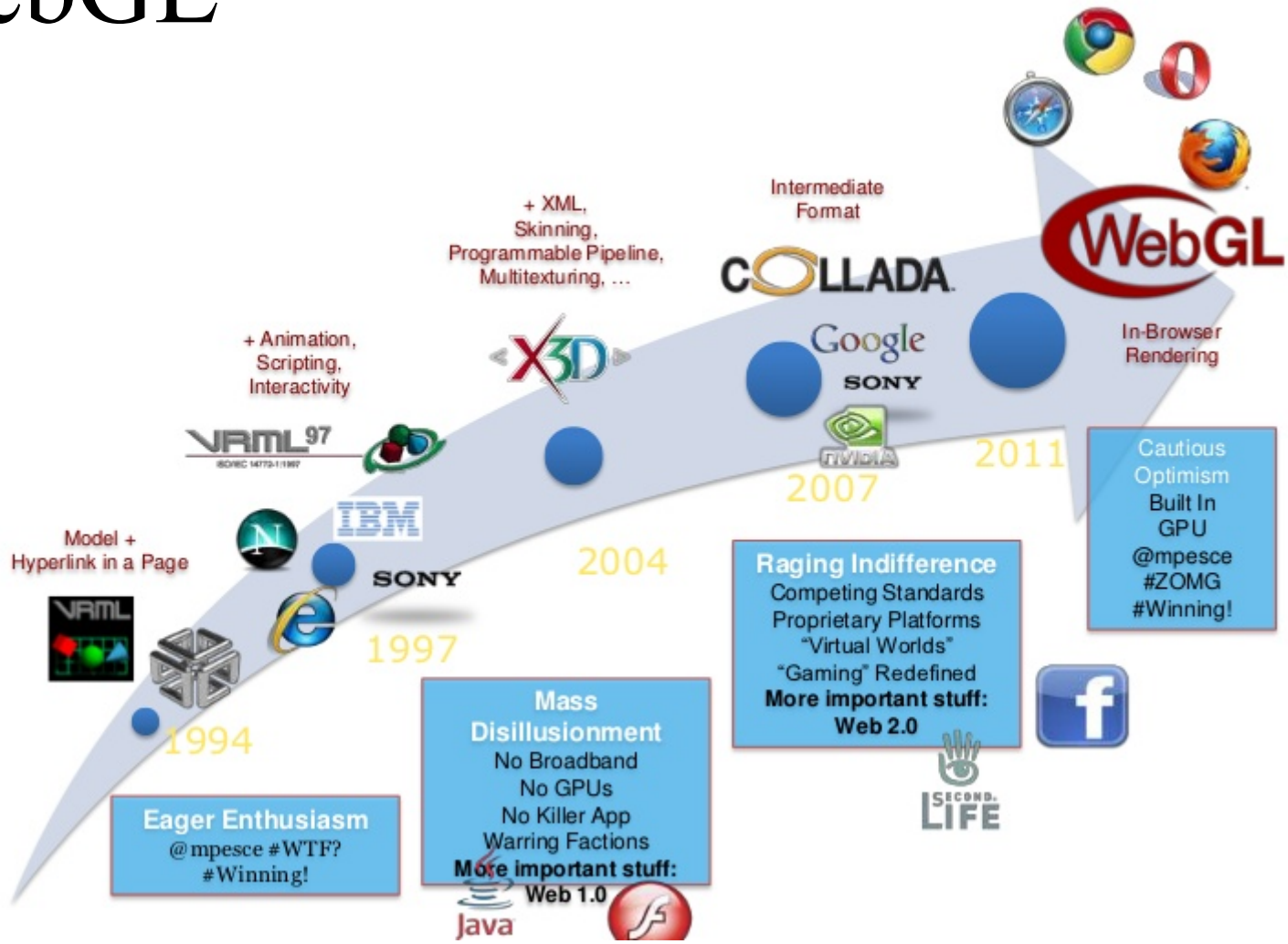
how to enable java in chrome? - Google Product Forums
productforums.google.com/d/topic/chrome/YjYREbIZoyc
Feb 26, 2012 - 73 posts - 49 authors
If you type "**java**" into the search settings, you'll be taken to "javascript". After updating to a fresh **chrome** and installing **java**, the **applets** are still saying you need to install **java**. When you navigate to the "test **java** installation" page, even that says you need **java**. This tells me that **Java** is not being enabled on ...

Enabling Java Runtime Environment (JRE) in Chrome 42
https://www.cas.org/products/chrome42-jre
Instructions for enabling **Java** Runtime Environment in **Chrome** 42.

Java …



WebGL

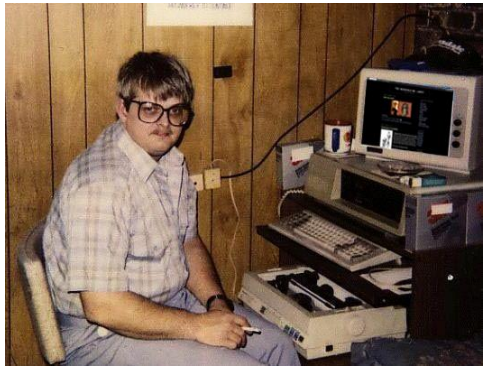


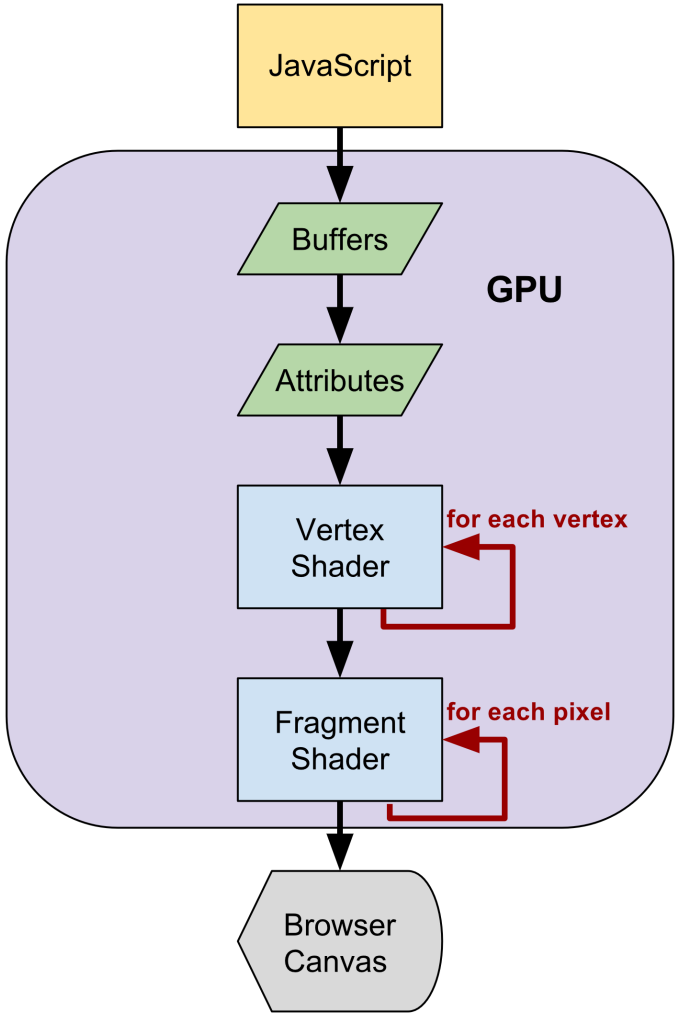
Remi Arnaud

WebGL

```
1  <html>
2  ...
3  <canvas></canvas>
4  ...
5  </html>
```

```
1  <script>
2  ...
3  let ctx = canvas.getContext('webgl');
4  ...
5  </script>
```

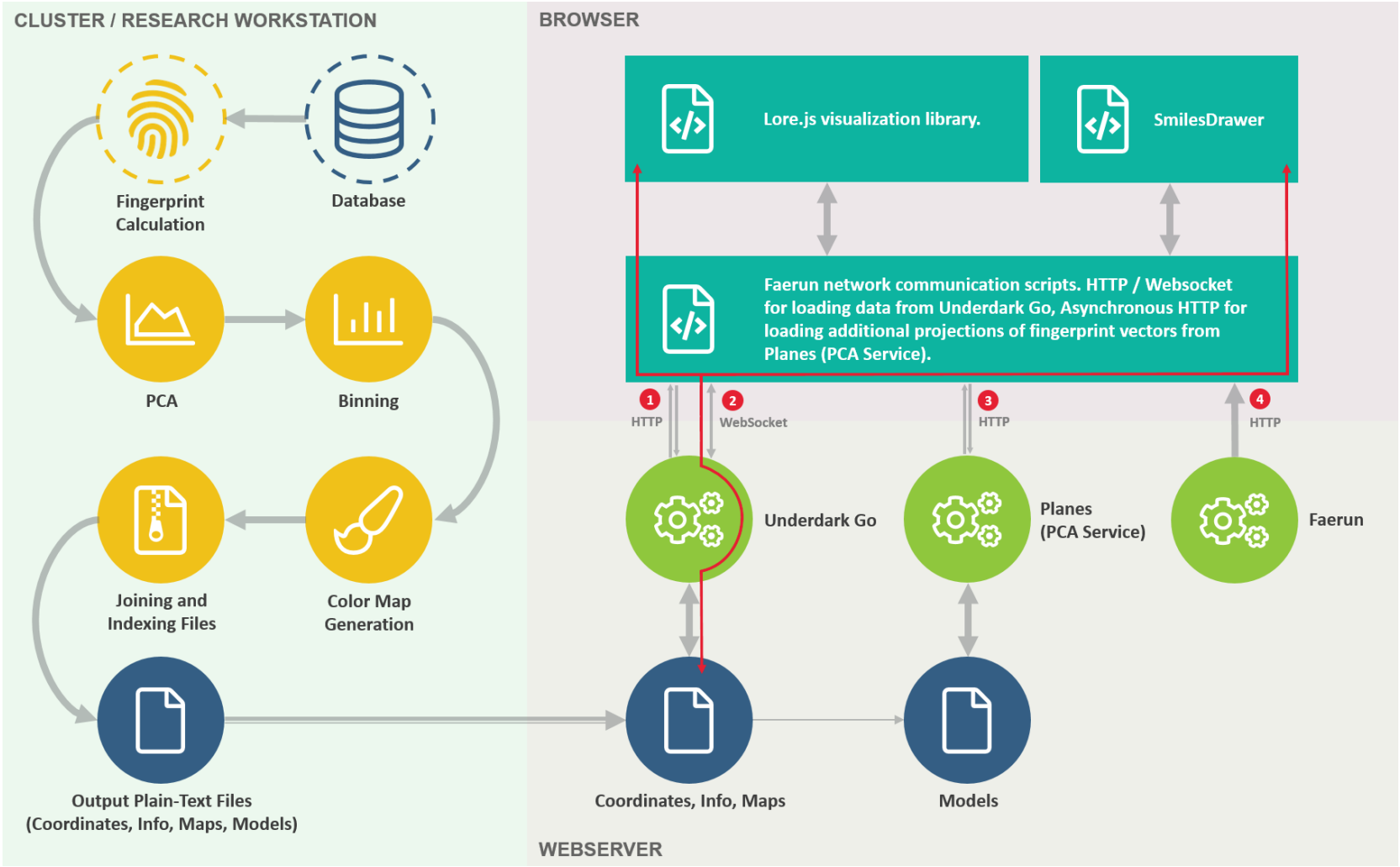


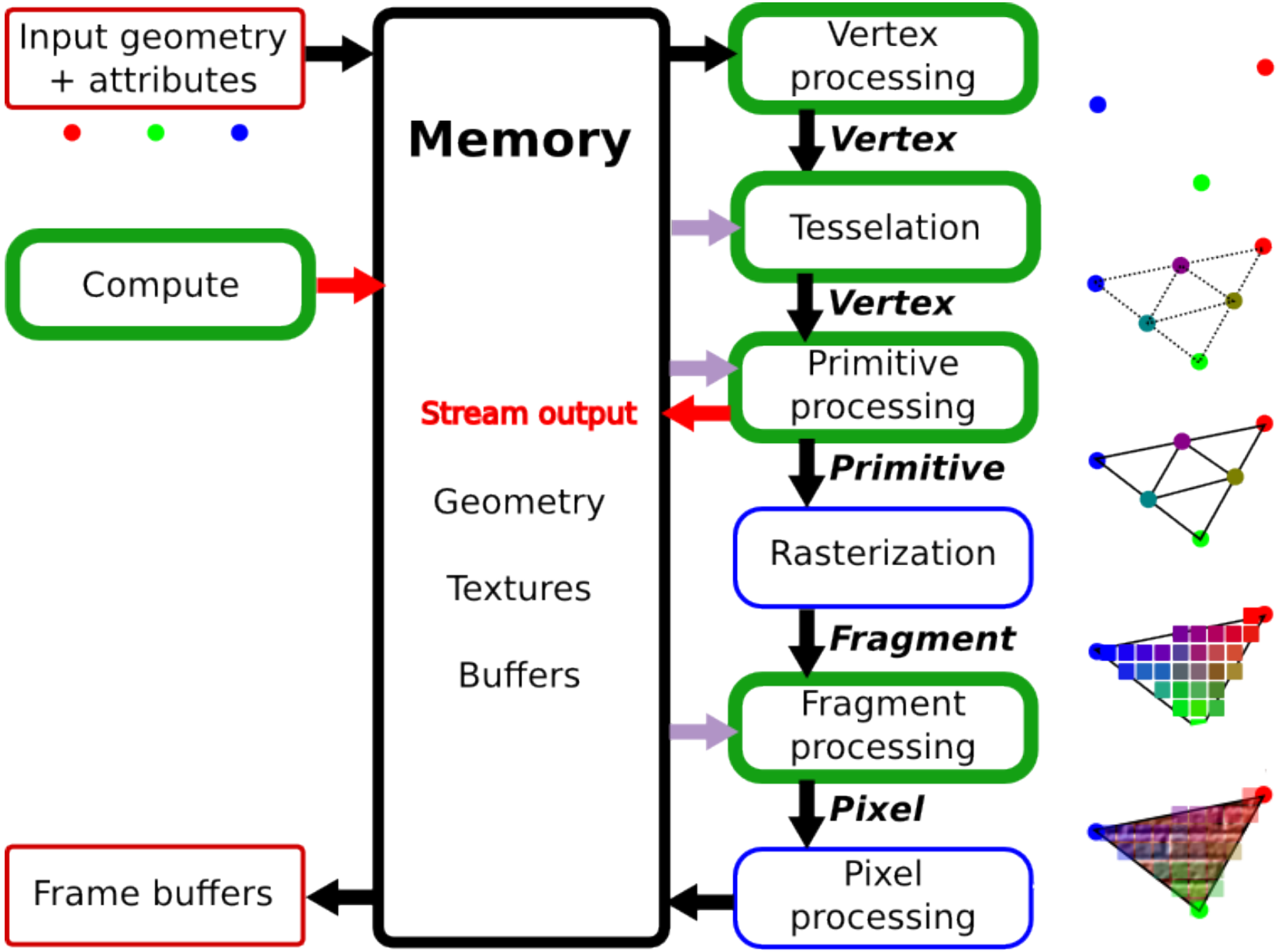


https://jsfiddle.net/greggman/8djzyjL3/

Brandon Rice

Faerun


CLUSTER / RESEARCH WORKSTATION
Fingerprint Calculation
Database
PCA
Binning
Joining and Indexing Files
Color Map Generation
Output Plain-Text Files (Coordinates, Info, Maps, Models)
BROWSER
Lore.js visualization library.
SmilesDrawer
Faerun network communication scripts. HTTP / Websocket for loading data from Underdark Go, Asynchronous HTTP for loading additional projections of fingerprint vectors from Planes (PCA Service).
1 HTTP
2 WebSocket
3 HTTP
4 HTTP
Underdark Go
Planes (PCA Service)
Faerun
Coordinates, Info, Maps
Models
WEBSERVER


Input geometry
+ attributes
Compute
Frame buffers
Memory
Stream output
Geometry
Textures
Buffers
Vertex
processing
Vertex
Tesselation
Vertex
Primitive
processing
Primitive
Rasterization
Fragment
Fragment
processing
Pixel
Pixel
processing