Scientific Visualization Basics

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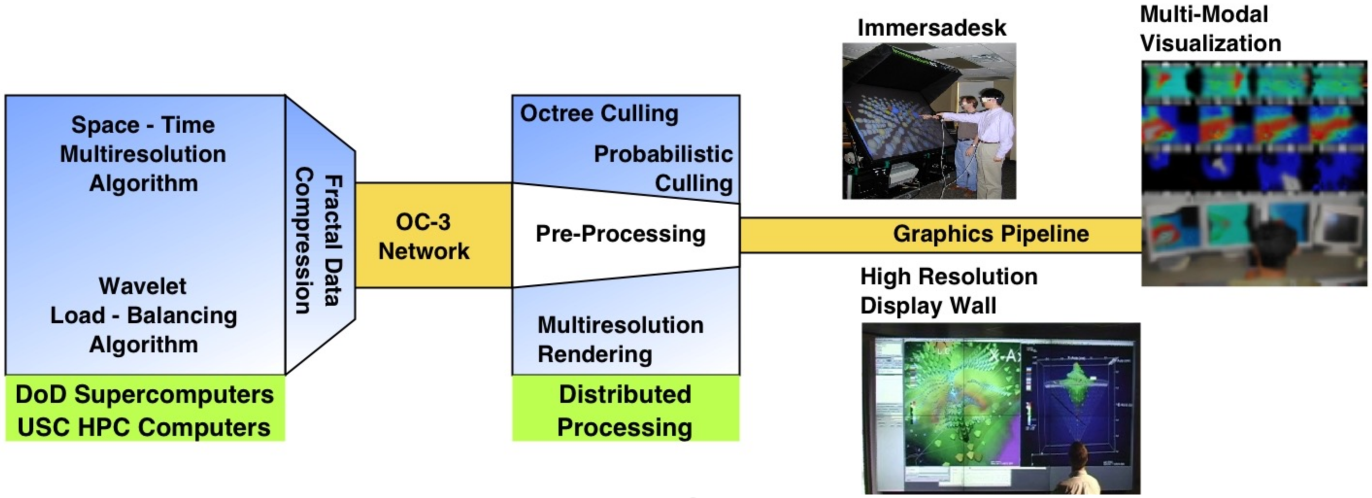
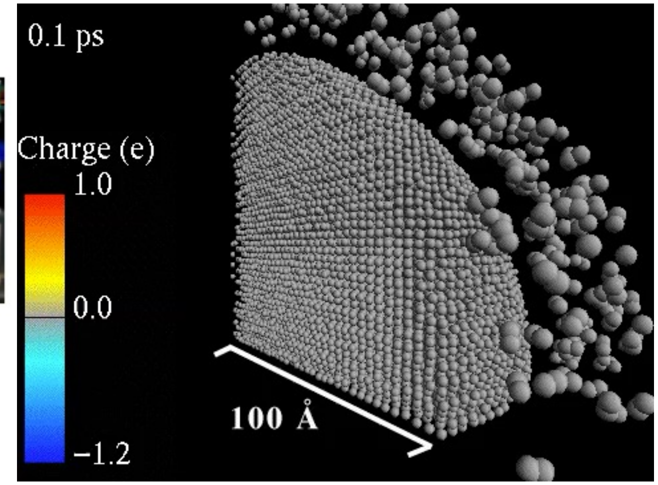
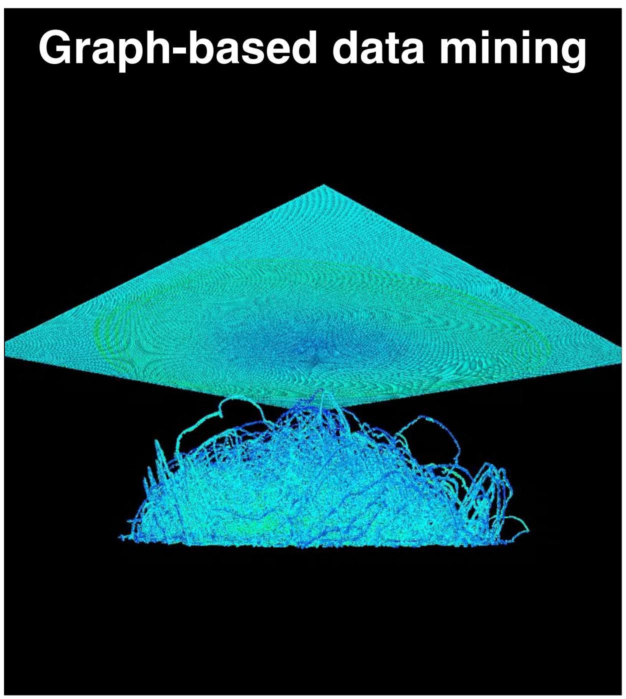
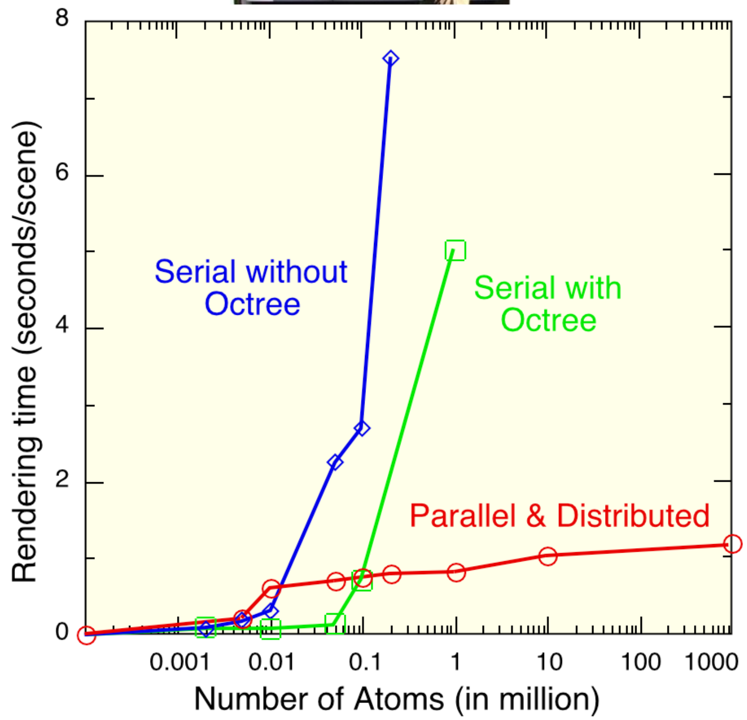
Goal: Experience simple OpenGL visualization of real simulation

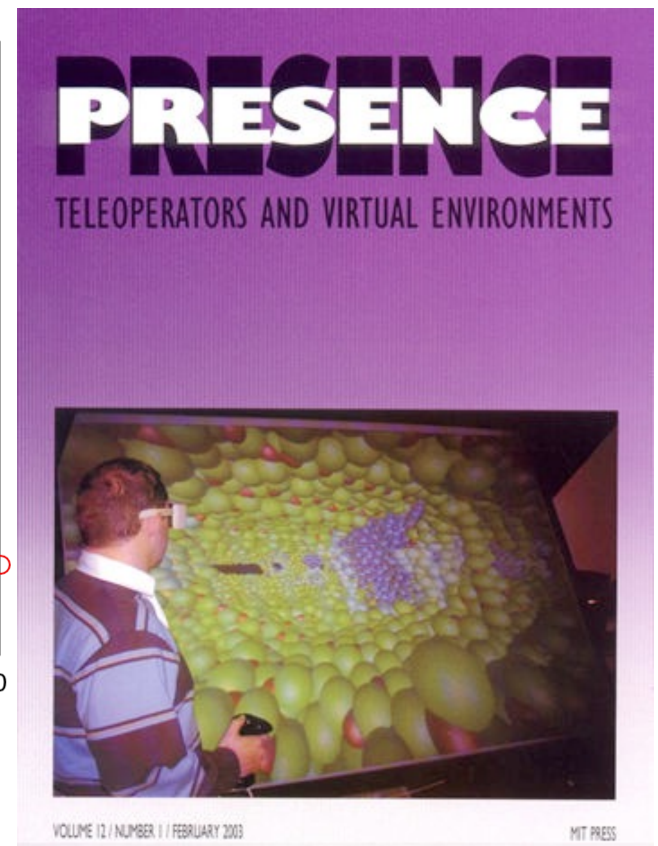
Massive Scientific Data Visualization











Interactive visualization of billion atoms

OpenGL: Getting Started

Installing OpenGL & GLUT libraries:

- **OpenGL: Standard, hardware-independent interface to graphics hardware.**
- **GLUT (OpenGL Utility Toolkit): Window-system-independent toolkit for window APIs.**

http://www.opengl.org

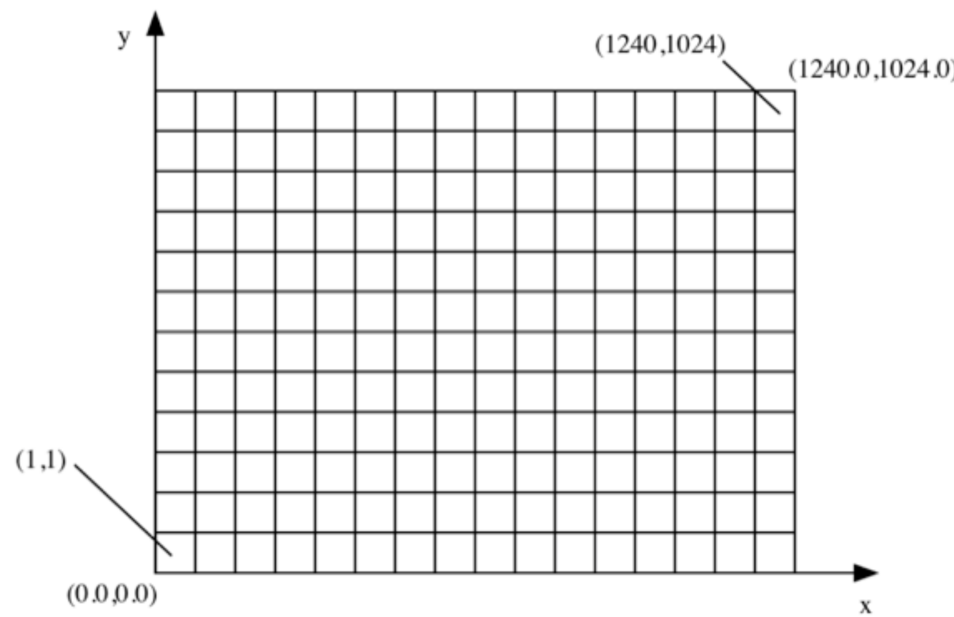
Do it on your laptop!

http://web.eecs.umich.edu/~sugih/courses/eecs487/glut-howto

OpenGL Programming Basics

```
#include <OpenGL/gl.h>     // Header File For The OpenGL32 Library
#include <OpenGL/glu.h>    // Header File For The GLu32 Library
#include <GLUT/glut.h>     // Header File For The GLut Library

glutInit(&argc, argv);

/* Set up an window */
glutInitDisplayMode(GLUT_DOUBLE|GLUT_RGBA|GLUT_DEPTH); /*Initialize display mode*/
glutInitWindowSize(winx, winy); /* Specify window size */
glutCreateWindow("Lennard-Jones Atoms"); /* Open window */
glEnable(GL_DEPTH_TEST); /* Enable z-buffer for hidden surface removal */
glClear(GL_COLOR_BUFFER_BIT|GL_DEPTH_BUFFER_BIT); /* Clear the window */
```

- **Frame buffer:** A collection of buffers in memory, which store data for screen pixels (*e.g.*, 1280 pixels wide & 1024 pixels high) such as color, depth information for hidden surface removal, *etc*.



https://aiichironakano.github.io/cs653/src/viz/ → atomv.c

OpenGL Event-Handling Loop

```
main() {
   /* Set a glut callback functions */
   glutDisplayFunc(display);
   glutReshapeFunc(reshape);
   /* Start main display loop */
   glutMainLoop();
}

/* Definition of callback functions */
display() {...}
reshape() {...}
```

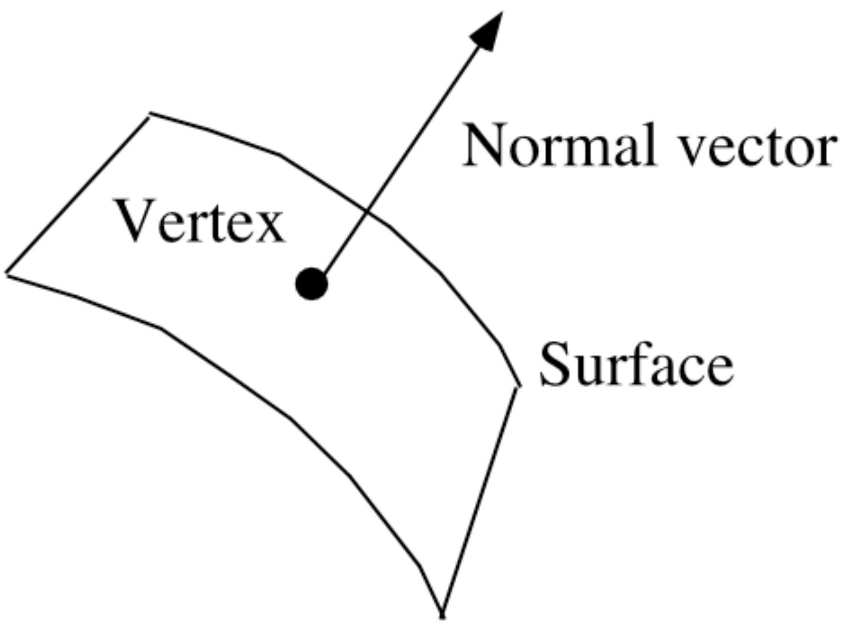
events

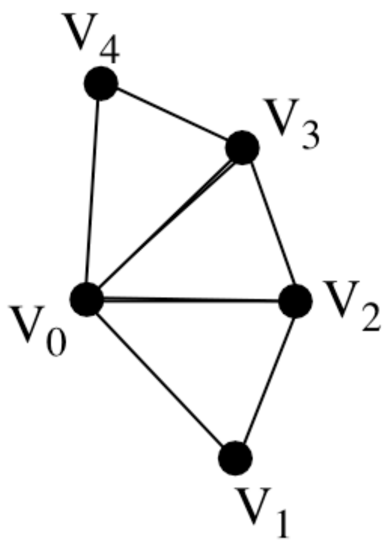
event handlers

Glut runtime system keeps listening if any event happens; when an even happens, it invokes the corresponding user-specified event handler function.

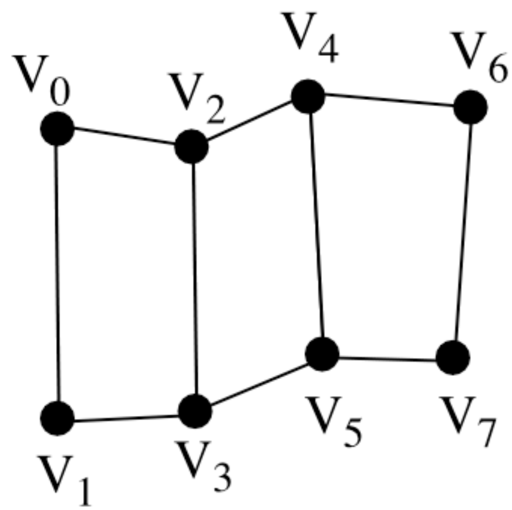
Polygonal Surfaces

```
float normal_vector[MAX_VERTICES][3],vertex_position[MAX_VERTICES][3];
glBegin(GL_QUAD_STRIP);
  for (i=0; i<number_of_vertices; i++) {
    glNormal3f(normal_vector[i]);
    glVertex3f(vertex_position[i]);
  }
glEnd();
```





GL_TRIANGLE_FAN

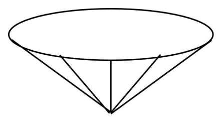


GL_QUAD_STRIP

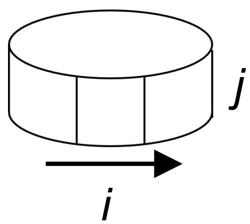
Polygonal Sphere

```
int nlon=18, nlat=9;
loninc = 2*M_PI/nlon; /* Δϕ */
latinc = M_PI/nlat;   /* Δθ */
/* South-pole triangular fan */
glBegin(GL_TRIANGLE_FAN);
  glNormal3f(0,-1,0);
  glVertex3f(0,-radius,0);
  lon = 0;
  lat = -M_PI/2 + latinc;
  y = sin(lat);
  for (i=0; i<=nlon; i++) {
    x = cos(lon)*cos(lat);
    z = -sin(lon)*cos(lat);
    glNormal3f(x,y,z);
    glVertex3f(x*radius,y*radius,z*radius);
    lon += loninc;}
glEnd();
```

south
bowl

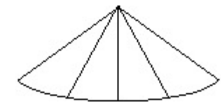


```
/* Quadrilateral strips to cover the sphere */
for (j=1; j<nlat-1; j++) {
  lon = 0;
  glBegin(GL_QUAD_STRIP);
    for (i=0; i<=nlon; i++) {
      x = cos(lon)*cos(lat);
      y = sin(lat);
      z = -sin(lon)*cos(lat);
      glNormal3f(x,y,z);
      glVertex3f(x*radius,y*radius,z*radius);
      x = cos(lon)*cos(lat+latinc);
      y = sin(lat+latinc);
      z = -sin(lon)*cos(lat+latinc);
      glNormal3f(x,y,z);
      glVertex3f(x*radius,y*radius,z*radius);
      lon += loninc;}
  glEnd();
  lat += latinc;}
```

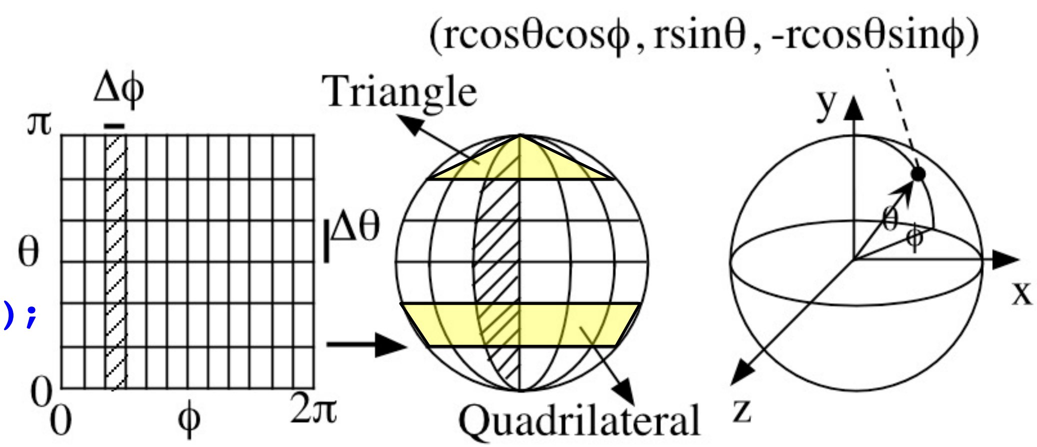



```
/* North-pole triangular fan */
glBegin(GL_TRIANGLE_FAN);
  glNormal3f(0,1,0);
  glVertex3f(0,radius,0);
  y = sin(lat);
  lon = 0;
  for (i=0; i<=nlon; i++) {
    x = cos(lon)*cos(lat);
    z = -sin(lon)*cos(lat);
    glNormal3f(x,y,z);
    glVertex3f(x*radius,y*radius,z*radius);
    lon += loninc;
  }
glEnd();
```

north
cap



Vertices in spherical → Cartesian coordinates



Display Lists

- **Display list:** A group of OpenGL commands that have been stored for later execution.

```
/* Generates one new display-list ID */
GLuint sphereid = glGenLists(1);

/* Define a routine to draw a sphere*/
glNewList(spherеid, GL_COMPILE);
  ...code to draw a sphere (previous slide)...
glEndList();

/* Execute sphere drawing */
glCallList(sphereid);
```

Transformation Matrix

Drawing spheres at many atom positions

- **Transformation matrix: Specifies the amount by which the object's coordinate system is to be rotated, scaled, or translated, *i.e.*, affine transformation.**

$$\overrightarrow{r'} = \overleftrightarrow{A}\vec{r} + \vec{b}$$

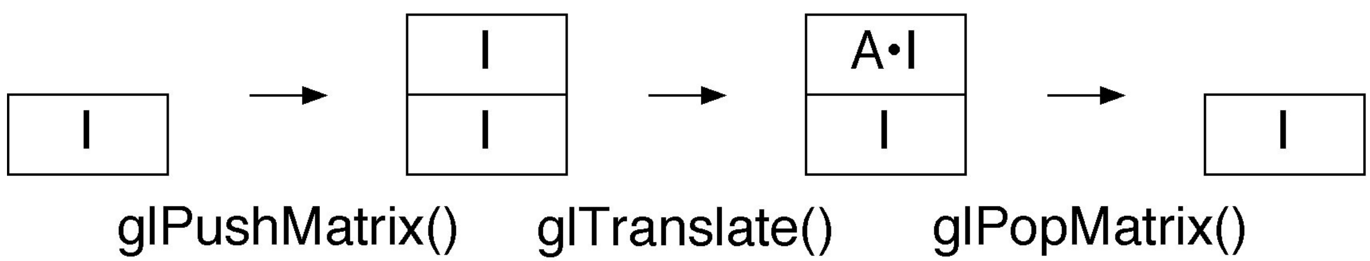
$$\begin{bmatrix} x' \\ y' \\ z' \\ 1 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix}$$

```
Matrix Identity
= {1, 0, 0, 0,
   0, 1, 0, 0,
   0, 0, 1, 0,
   0, 0, 0, 1};
```

- **Matrix stack: A stack of transformation matrices—at the top of the stack is the current transformation matrix applied to all vertices. Initially the transformation matrix is the identity matrix.**

```
glPushMatrix();
glTranslatef(atoms[i].crd[0],atoms[i].crd[1],atoms[i].crd[2]);
glCallList(sphereid);
glPopMatrix();
```

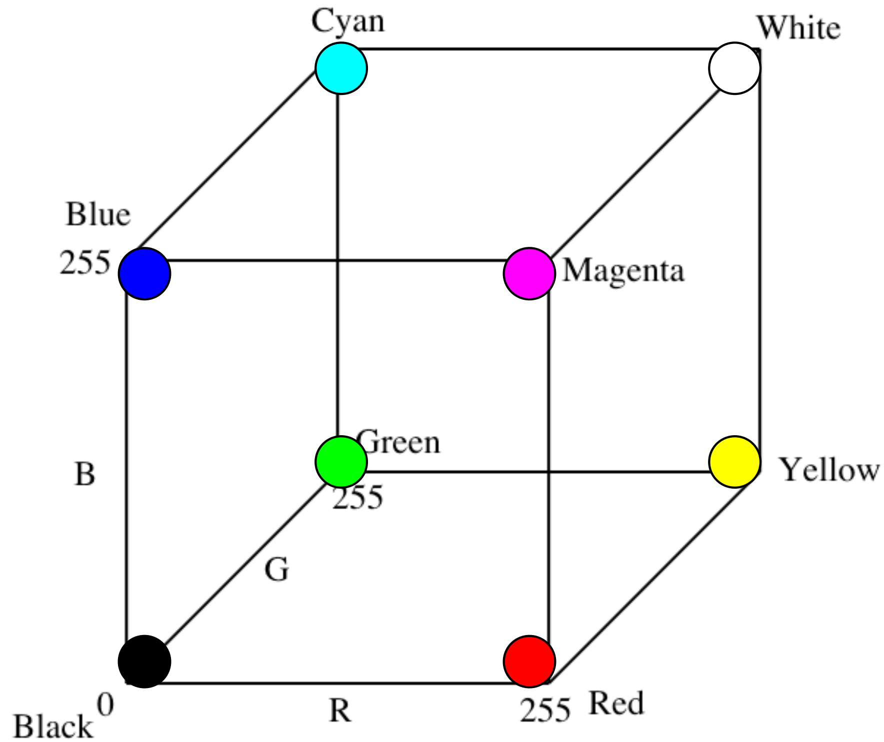
Repeat this *nAtom* times



Color Display

- **RGB(A) mode:** Specifying color by providing red, green & blue intensities (& alpha component).
- **Alpha component:** Specifies the opacity of a material; default value is 1.0 (nontransparent), if not specified.

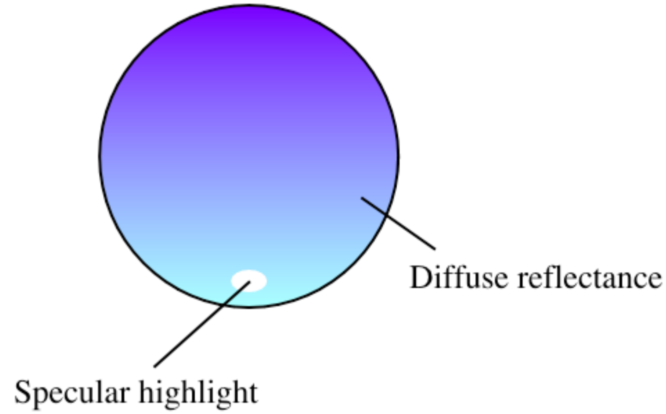
```
float r=1.0; g=0.0; b=0.0;

glColor3f(r,g,b);
```



- **OpenGL as a state machine:** Color change stays.

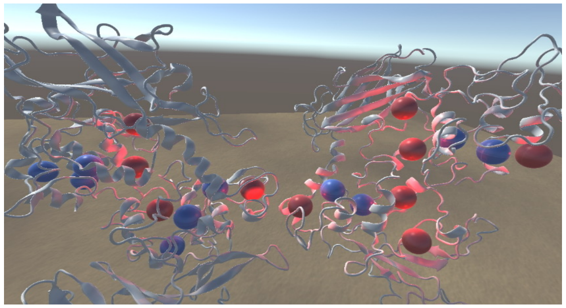
Lighting & Materials

OpenGL color =
light × material-reflectance



OpenGL Color Types

- **Diffuse component:** Gives the appearance of a matter or flat reflection from an object's surface.
- **Ambient illumination:** Simulates light reflected from other objects.
- **Specular light:** Creates highlights.
- **Emission:** Simulates the appearance of lights in the scene.



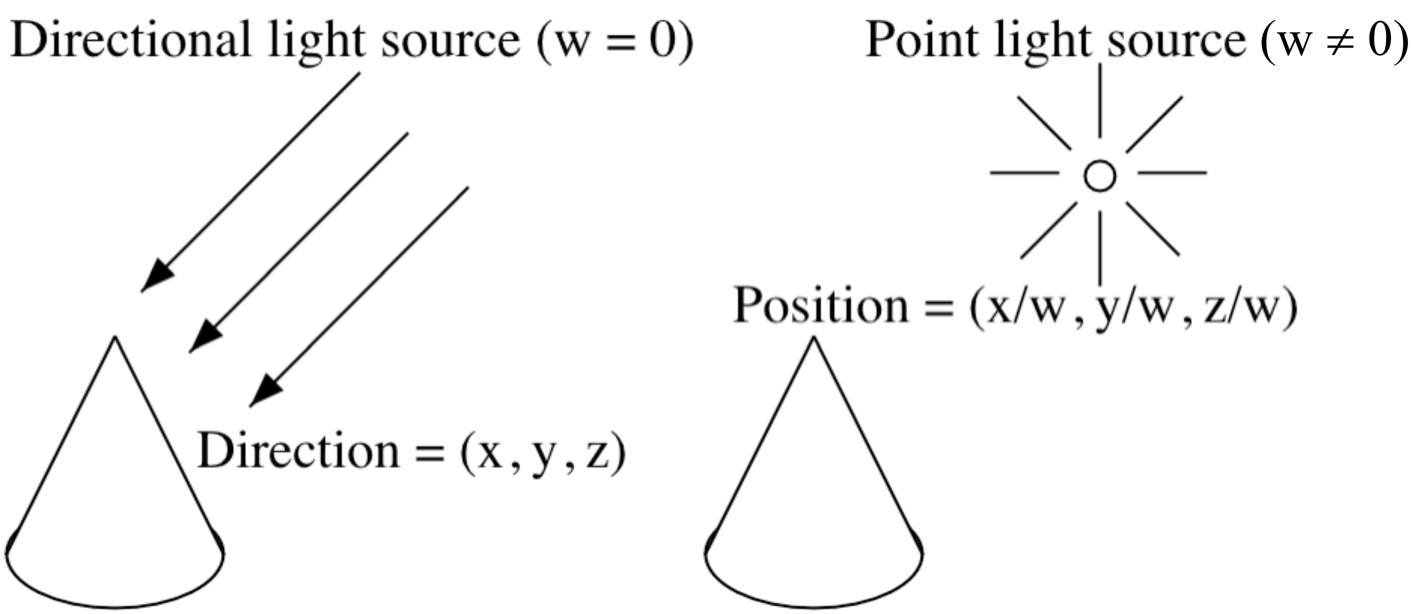
Materials Definition

- **Refelectance:** Material is characterized by ambient, diffuse & specular reflectance, *i.e.*, how the object reflects light.
- `glEnable(GL_COLOR_MATERIAL)`
  In this mode, the current color specified by `glColor*()` will change the ambient & diffuse reflectance.

Lighting Source

color = light × material (*e.g.*, $\alpha = \alpha_{light} \times \alpha_{material}$)

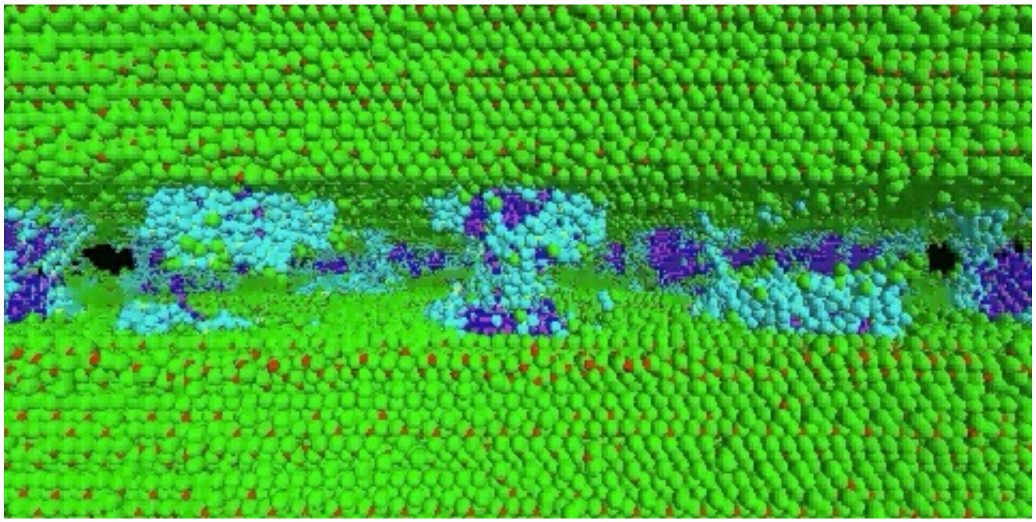
```
float light_diffuse[4] = {1.0,1.0,1.0,1.0};
float light_position[4] = {0.5,0.5,1.0,0.0};

/* Define a lighting source */
glLightfv(GL_LIGHT0,GL_DIFFUSE,light_diffuse);
glLightfv(GL_LIGHT0,GL_POSITION,light_position);

/* Enable a single OpenGL light */
glEnable(GL_LIGHTING);
glEnable(GL_LIGHT0);
```

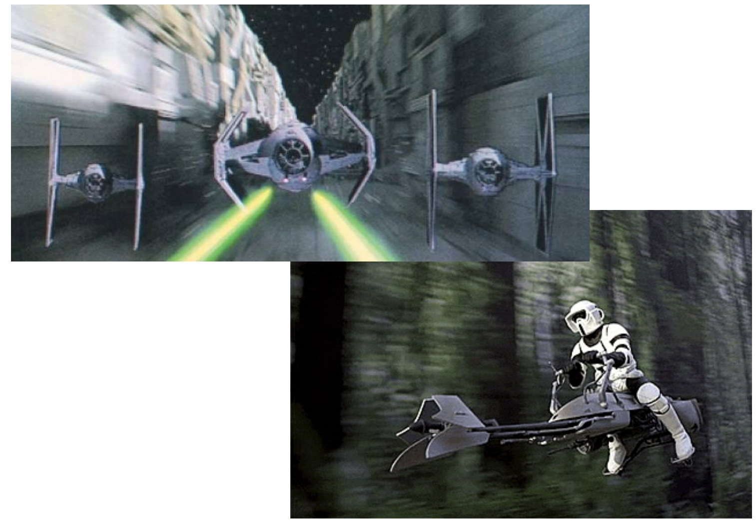


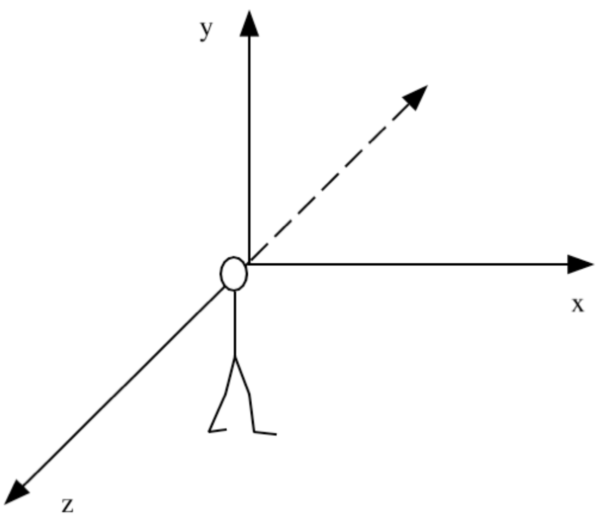
Viewing Transformation

- **Viewing transformation:** **Transforms object coordinates to eye coordinates.**

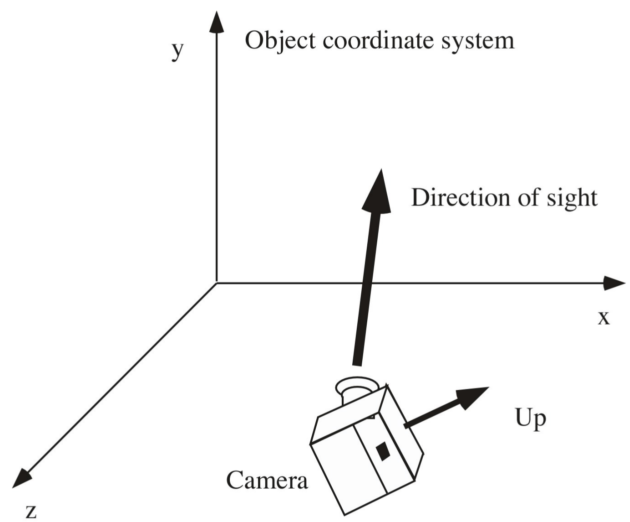
```
gluLookat(eyx, eyey, eyz, centerx, centery, centerz, upx, upy, upz);
```







Eye coordinate system

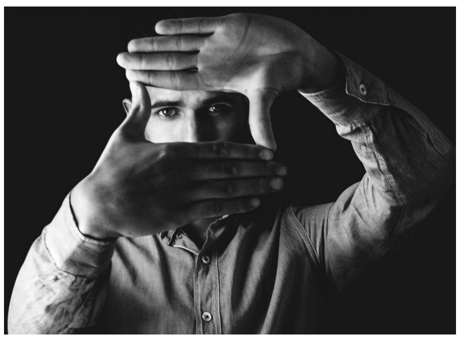


Camera specification

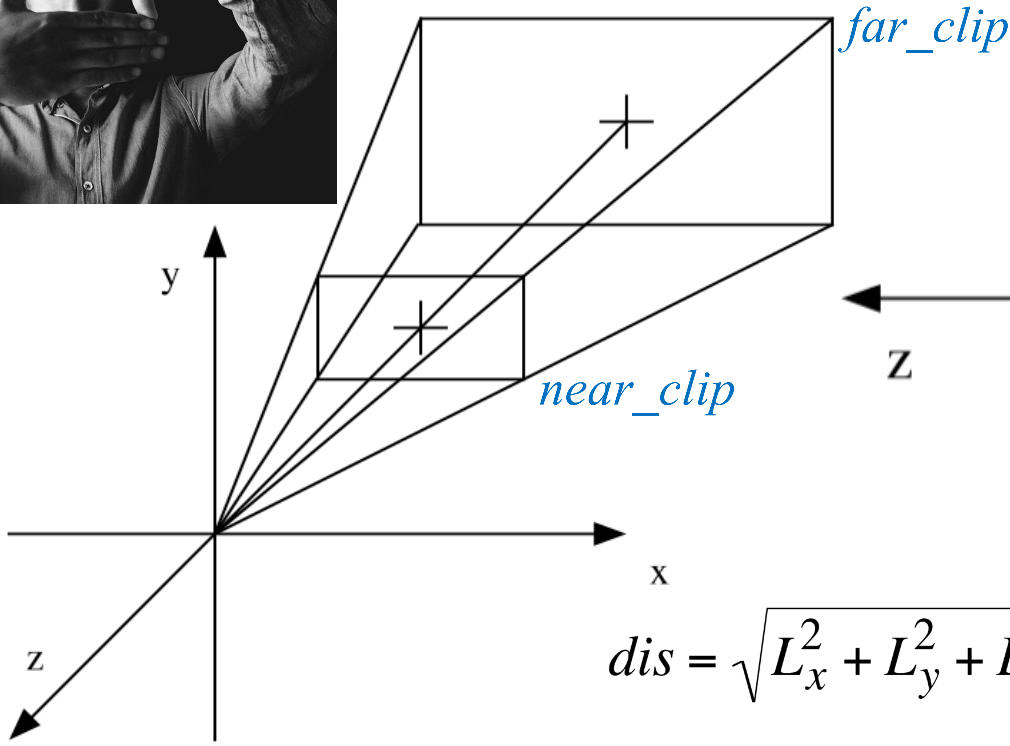
Clipping

```
void reshape (int w, int h) {
  ...
  /* set the GL viewport to match the full size of the window */
  glViewport(0, 0, (GLsizei)w, (GLsizei)h);
  aspect = w/(float)h;
  glMatrixMode(GL_PROJECTION);
  glLoadIdentity();
  gluPerspective(fovy,aspect,near_clip,far_clip);
  glMatrixMode(GL_MODELVIEW);
}
```

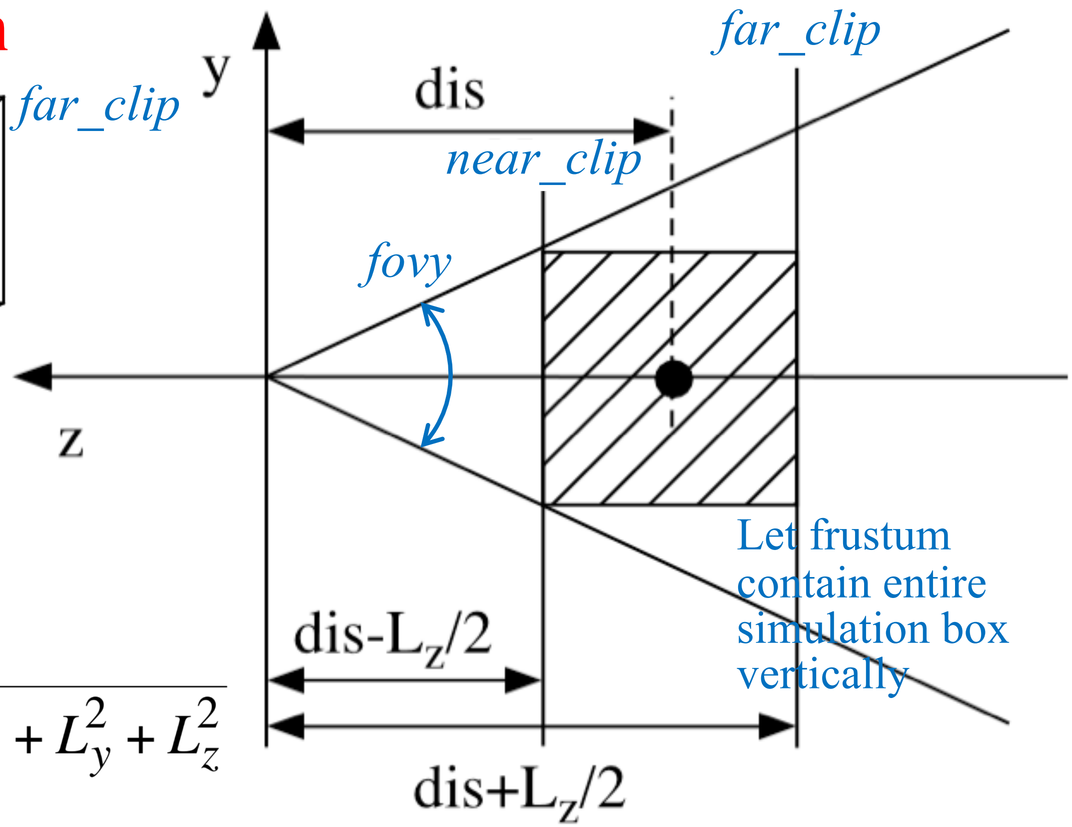
$$fovy = 2\tan^{-1}\left(\frac{L_y/2}{dis - L_z/2}\right)$$



View Frustum

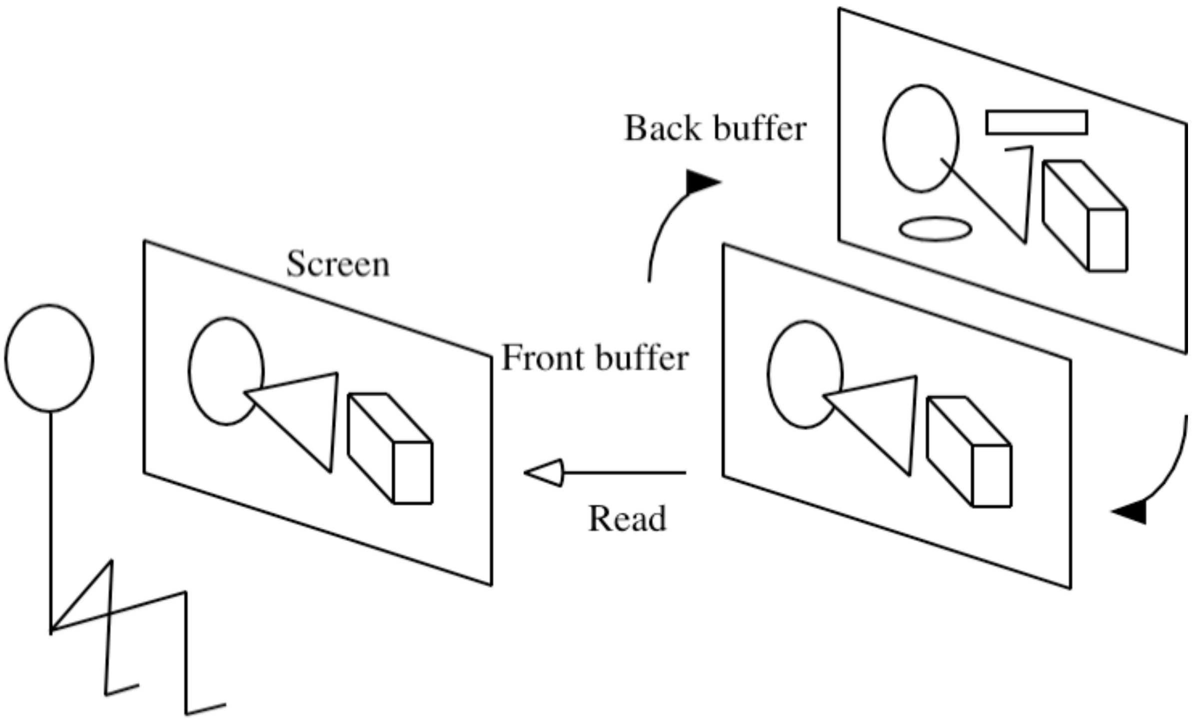


$$dis = \sqrt{L_x^2 + L_y^2 + L_z^2}$$



Animation

```
main() {
  glutIdleFunc(animate);
}
...
void animate() { /* Callback function for idle events */
/* Keep updating the scene until the last MD step is reached */
  if (stepCount <= StepLimit) {
    SingleStep(); /* One MD-step integration */
    if (stepCount%StepAvg == 0) EvalProps();
    makeCurframeGeom(); /* Redraw the scene */
    glutPostRedisplay();
    ++stepCount;
  }
}
```

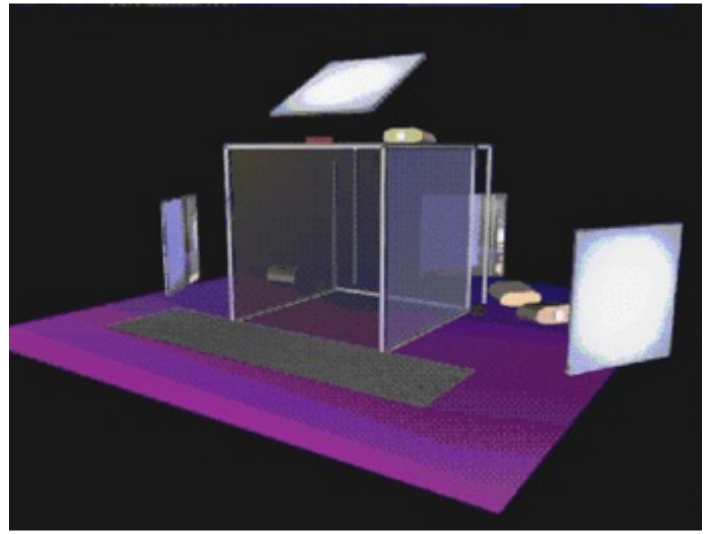


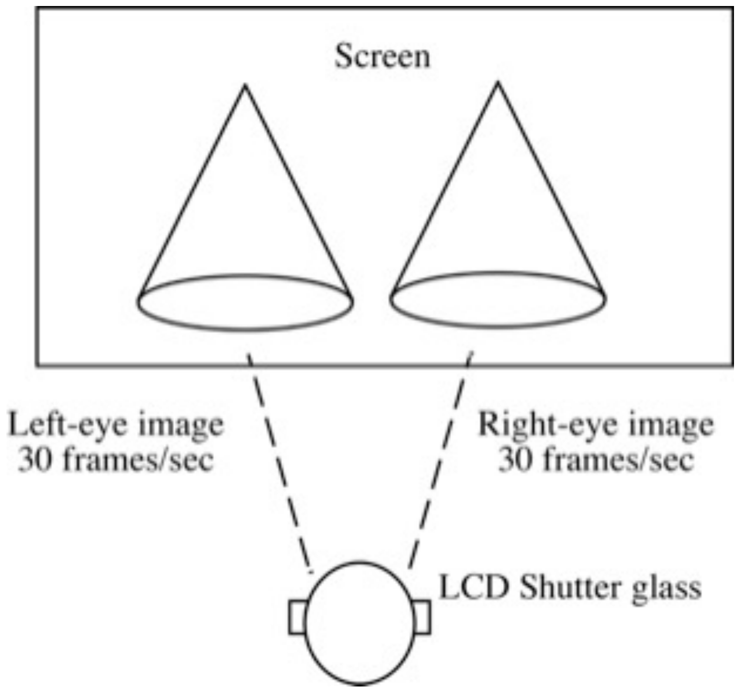

```
void display() {
  ...
  drawScene();
  glutSwapBuffers();
}
```

Immersive & Interactive Visualization

ImmersaDesk at CACS

CAVE





- **Stereographics**
- **Tracking system**
- **Wand: 3D (6 degrees-of-freedom) mouse**

Origin: Sutherland (1968)

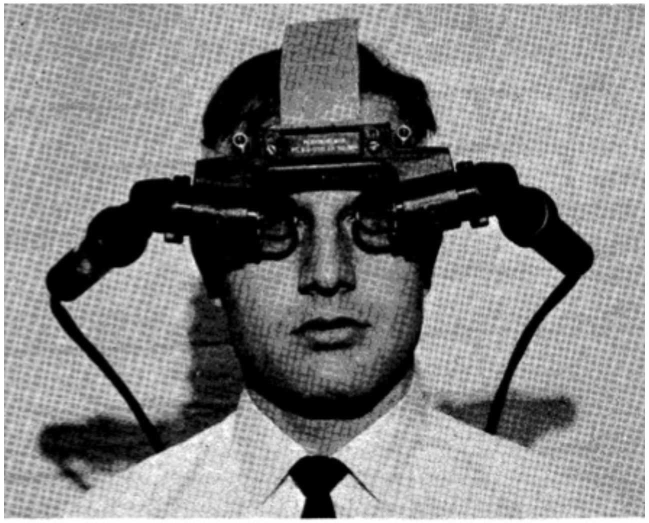


FIGURE 2—The head-mounted display optics with miniature CRT's

FIGURE 4—The ultrasonic head position sensor in use

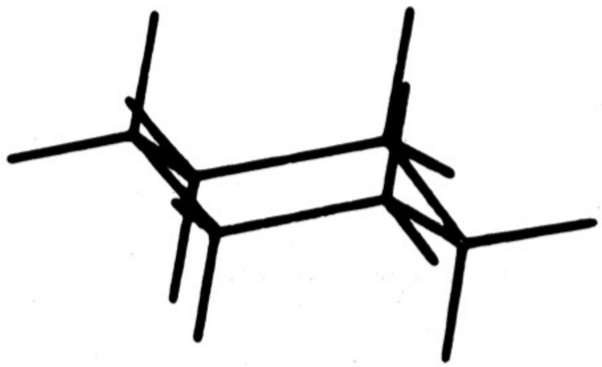


FIGURE 8—A computer-displayed perspective view of the cyclo-hexane molecule

Scientific VR

Journal of Molecular Graphics and Modelling 65 (2016) 94–99

Contents lists available at ScienceDirect

Journal of Molecular Graphics and Modelling

journal homepage: www.elsevier.com/locate/JMGM

ELSEVIER

iBET: Immersive visualization of biological electron-transfer dynamics

CrossMark

C. Masato Nakano [a], Erick Moen [b], Hye Suk Byun [c], Heng Ma [d], Bradley Newman [e], Alexander McDowell [e], Tao Wei [d,*], Mohamed Y. El-Naggar [c,f,g,**]

SoftwareX 9 (2019) 112–116

Contents lists available at ScienceDirect

SoftwareX

journal homepage: www.elsevier.com/locate/softx

ELSEVIER

Original software publication

Game-Engine-Assisted Research platform for Scientific computing (GEARS) in Virtual Reality

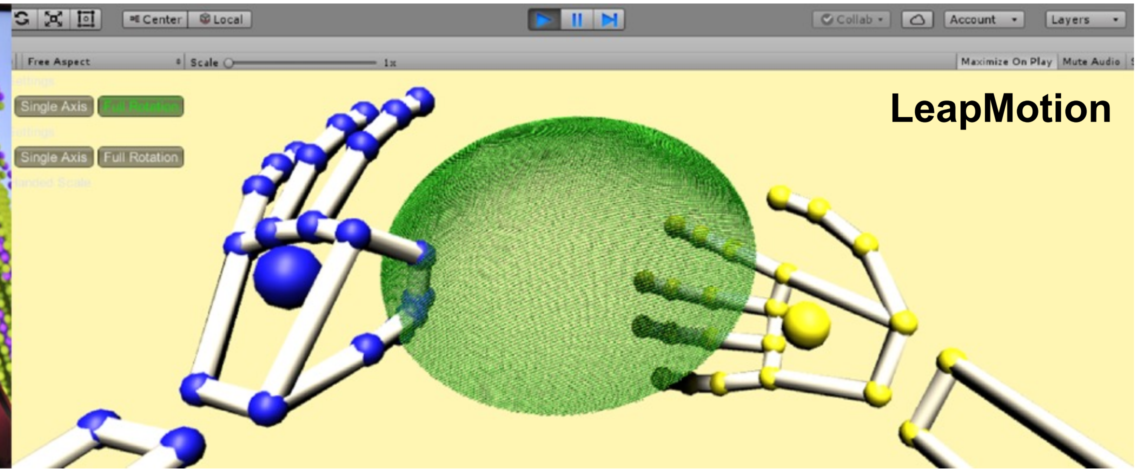
Brandon K. Horton [a], Rajiv K. Kalia [a,b,c,d], Erick Moen [b,e], Aiichiro Nakano [a,b,c,d,f], Ken-ichi Nomura [a,d,*], Michael Qian [a], Priya Vashishta [a,b,c,d], Anders Hafreager [g]

GEARS

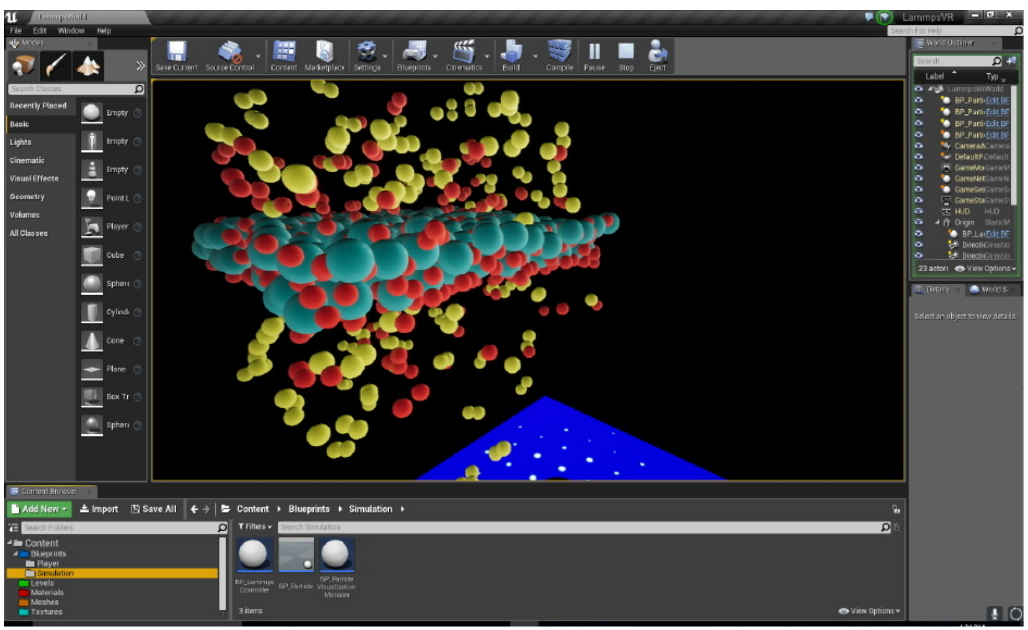
https://github.com/USCCACS/GEARS

Scientific VR Use Cases

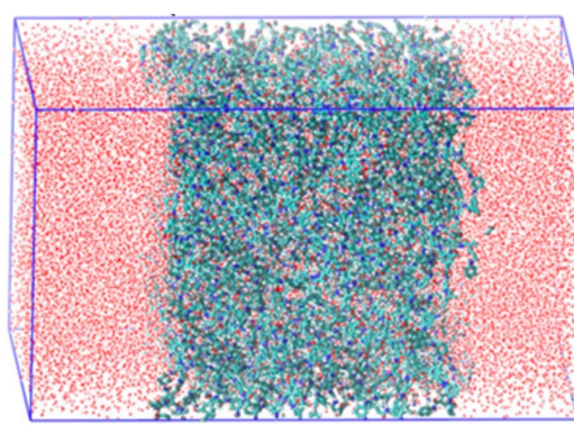
Interact with data



Dynamic linking to LAMMPS molecular-dynamics (MD) code



Virtual confocal microscopy



CAVE Library Programming

```
#include <cave_ogl.h>
#include <GL/glu.h>

GLUquadricObj *sphereObj;
void init_gl(void) {
 float redMaterial[] = { 1, 0, 0, 1 };
 glEnable(GL_LIGHT0);
 glMaterialfv(GL_FRONT_AND_BACK, GL_AMBIENT_AND_DIFFUSE, redMaterial);
 sphereObj = gluNewQuadric();
}

void draw_ball(void) {
 glClearColor(0., 0., 0., 0.);
 glClear(GL_DEPTH_BUFFER_BIT|GL_COLOR_BUFFER_BIT);
 glEnable(GL_LIGHTING);
 glPushMatrix();
 glTranslatef(0.0, 4.0, -4.0);
 gluSphere(sphereObj, 1.0, 8, 8);
 glPopMatrix();
 glDisable(GL_LIGHTING);
}
main(int argc,char **argv) {
 CAVEConfigure(&argc,argv,NULL); /* Initialize the CAVE */
 CAVEInit();
 CAVEInitApplication(init_gl,0); /* Pointer to the GL initialization function */
 CAVEDisplay(draw_ball,0); /* Pointer to the drawing function */
 while (!CAVEgetbutton(CAVE_ESCKEY)) /* Wait for the escape key to be hit */
   sginap(10); /* Nap so that this busy loop doesn't waste CPU time */
 CAVEExit(); /* Clean up & exit */
}
```

http://cacs.usc.edu/education/cs653.html → ball.c