

Visualizing Molecular Dynamics

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations

Department of Computer Science

Department of Physics & Astronomy

Department of Chemical Engineering & Materials Science

Department of Quantitative & Computational Biology

University of Southern California

Email: anakano@usc.edu

Goal: Visualize simulation to “understand” it

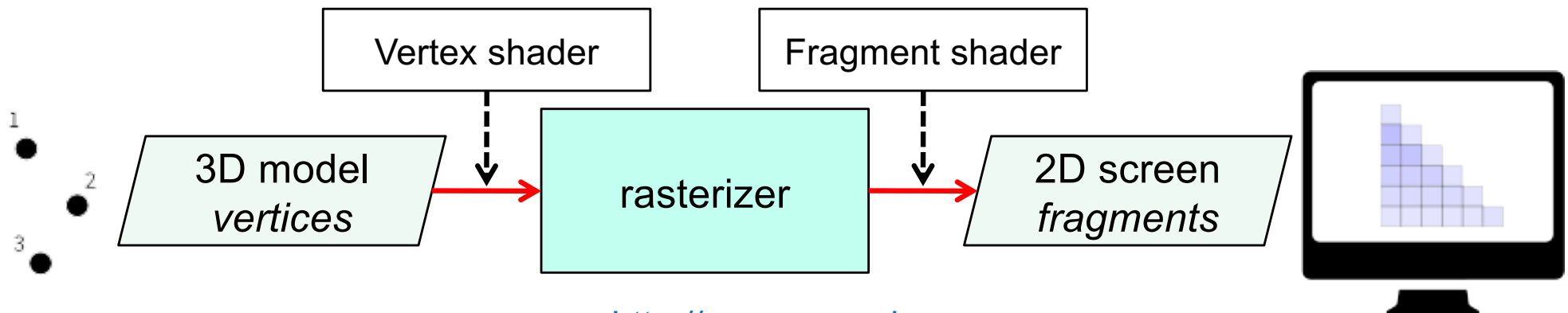


OpenGL: Getting Started

Installing OpenGL & GLUT libraries:

- **OpenGL (Open Graphics Language):** Standard, hardware-independent interface to graphics hardware.
- **GLUT (OpenGL Utility Toolkit):** Window-system-independent toolkit for window application programming interfaces (APIs). [How to install OpenGL & GLUT:
http://web.eecs.umich.edu/~sugih/courses/eecs487/glut-howto](http://web.eecs.umich.edu/~sugih/courses/eecs487/glut-howto)
- * This lecture describes basic graphics concepts common with earlier versions of OpenGL. In newer versions, shaders written in the **OpenGL Shading Language (GLSL)** determine various rendering attributes.

OpenGL rendering pipeline



<http://www.opengl.org>

OpenGL History

1992 OpenGL released by Silicon Graphics, Inc. (SGI)

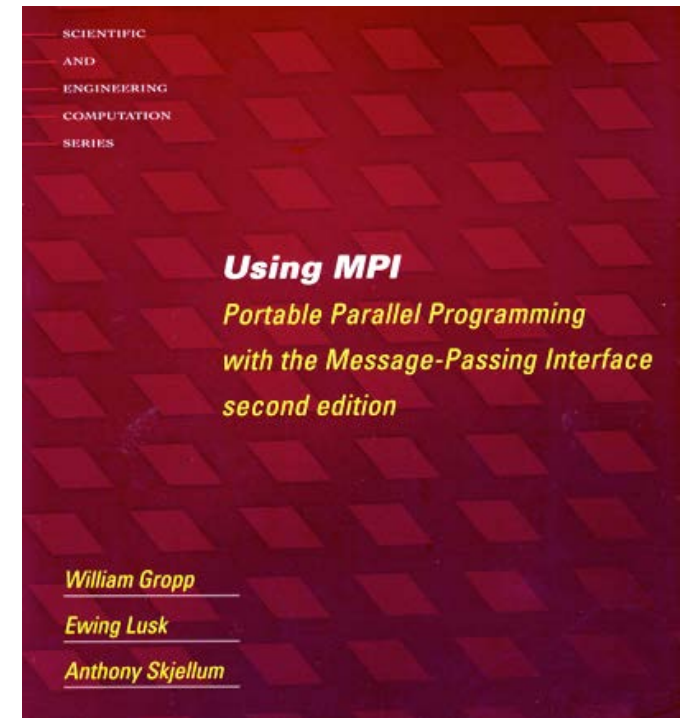
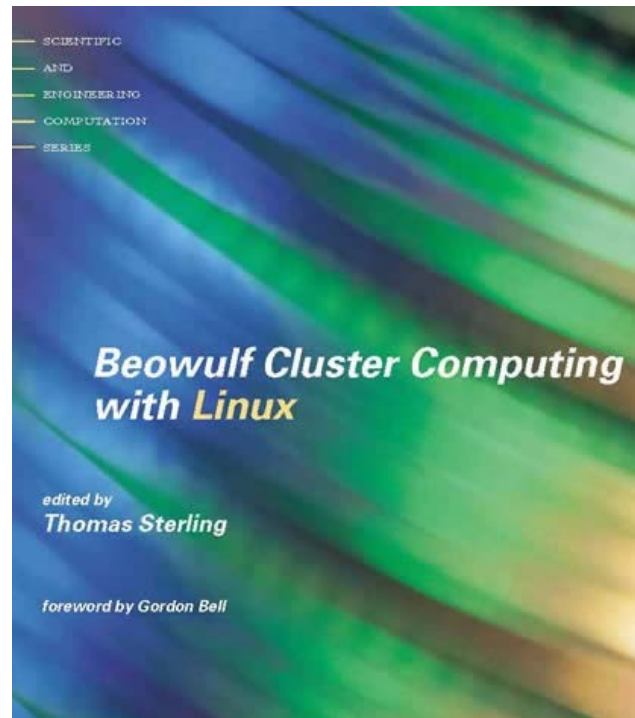
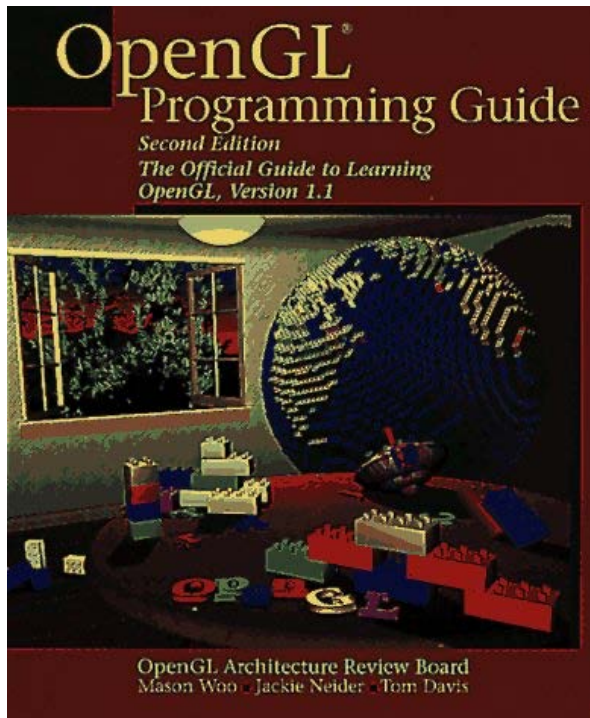
1994 Beowulf cluster computer
MPI 1.0 (message passing)
`MPI_Send()`, `MPI_Recv()`

1997 OpenMP 1.0 (multithreading)
`#pragma omp parallel`

2004 OpenGL2.0: OpenGL Shading Language (GLSL) included for controlling graphics cards

2008 OpenGL3.0: Major revision

2007 CUDA 1.0 (graphics cards)



OpenGL Programming Basics

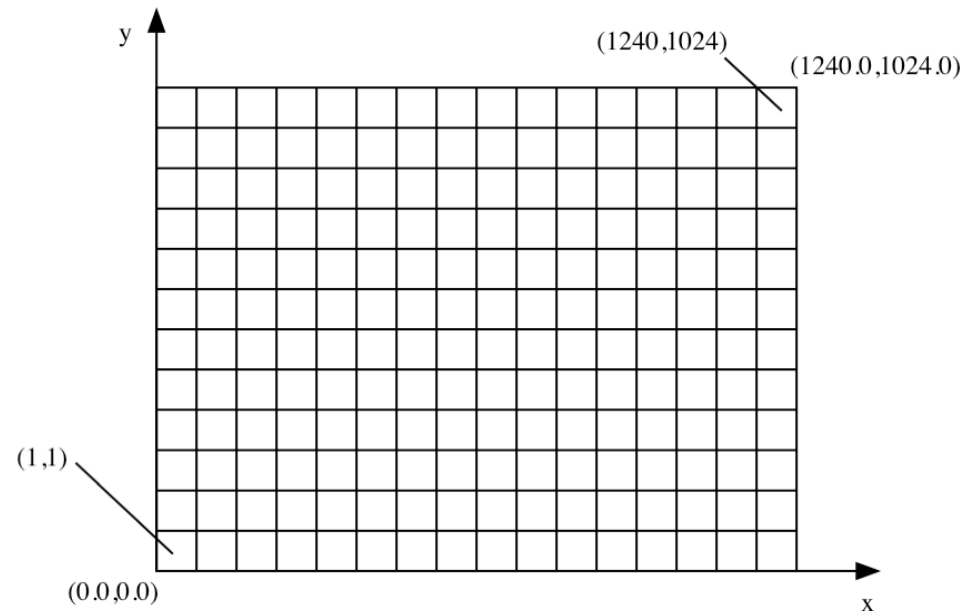
atomv.c (<https://aiichironakano.github.io/cs596/src/viz>)

```
#include <OpenGL/gl.h>      // Header File For The OpenGL Library
#include <OpenGL/glu.h>     // Header File For The GLu 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.*



OpenGL Event-Handling Loop

```
main() {  
    /* Set a glut callback functions */  
    glutDisplayFunc(display);  
    glutReshapeFunc(reshape);  events  
    /* Start main display loop */  
    glutMainLoop();  
}  
  
/* Definition of callback functions */  
display() {...}  
reshape() {...}  event handlers
```

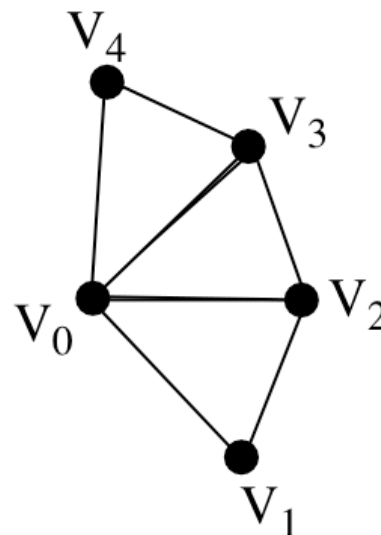
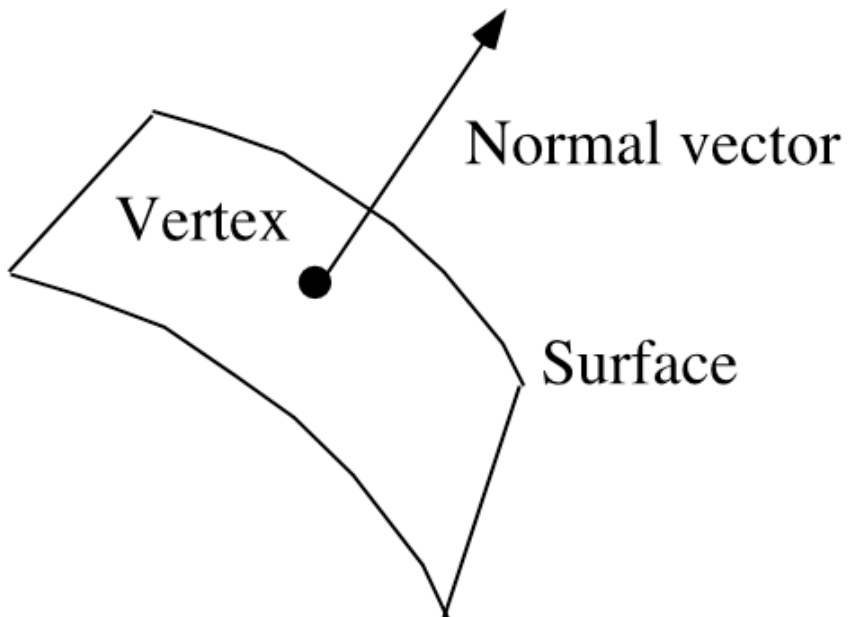
→ Glut runtime system keeps listening if any event happens; when an even happens, it invokes the corresponding user-specified event handler function.

All topics in this presentation are detailed in
<https://aiichironakano.github.io/cs596/Visual.pdf>

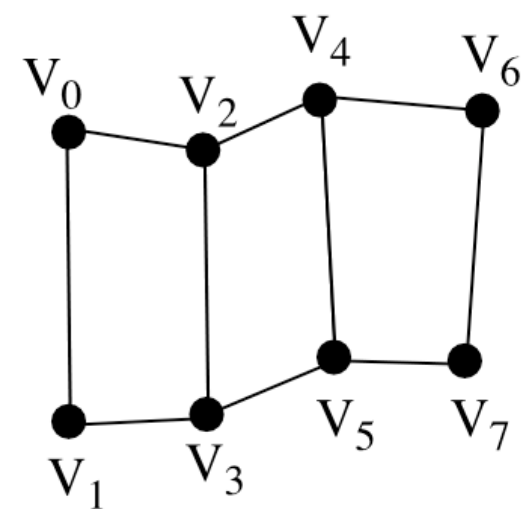
Polygonal Surfaces

Drawing a set of polygons

```
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

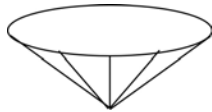


GL_QUAD_STRIP

Polygonal Sphere

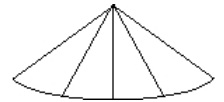
```
int nlon=18, nlat=9;
loninc = 2*M_PI/nlon; /*  $\Delta\phi$  */
latinc = M_PI/nlat;   /*  $\Delta\theta$  */
/* South-pole triangular fan */
glBegin(GL_TRIANGLE_FAN);
  glNormal3f(0,-1,0);
  glVertex3f(0,-radius,0);
  lon = 0;
  lat = -M_PI/2 + latinc;
  y = sin(lat);
  for (i=0; i<=nlon; i++) {
    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

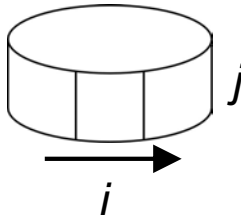


```
/* North-pole triangular fan */
glBegin(GL_TRIANGLE_FAN);
  glNormal3f(0,1,0);
  glVertex3f(0,radius,0);
  y = sin(lat);
  lon = 0;
  for (i=0; i<=nlon; i++) {
    x = cos(lon)*cos(lat);
    z = -sin(lon)*cos(lat);
    glNormal3f(x,y,z);
    glVertex3f(x*radius,y*radius,z*radius);
    lon += loninc;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

north
cap

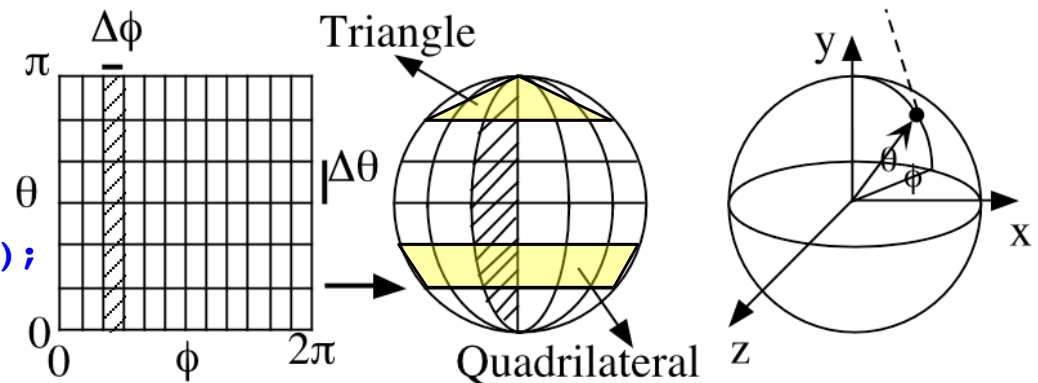


```
/* Quadrilateral strips to cover the sphere */
for (j=1; j<nlat-1; j++) {
  lon = 0;
  glBegin(GL_QUAD_STRIP);
  for (i=0; i<=nlon; i++) {
    x = cos(lon)*cos(lat);
    y = sin(lat);
    z = -sin(lon)*cos(lat);
    glNormal3f(x,y,z);
    glVertex3f(x*radius,y*radius,z*radius);
    x = cos(lon)*cos(lat+latinc);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



Vertices in spherical \rightarrow Cartesian coordinates

$(r\cos\theta\cos\phi, r\sin\theta, -r\cos\theta\sin\phi)$



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(sphereid, 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**.

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

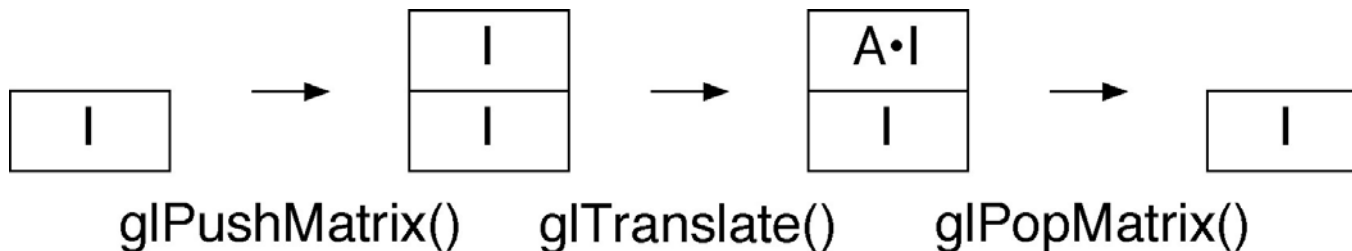
$$\begin{bmatrix} x' \\ y' \\ z' \\ 1 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix}$$

$$\begin{aligned} &\text{Matrix Identity} \\ &= \{1, 0, 0, 0, \\ &\quad 0, 1, 0, 0, \\ &\quad 0, 0, 1, 0, \\ &\quad 0, 0, 0, 1\}; \end{aligned}$$

- 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();
```

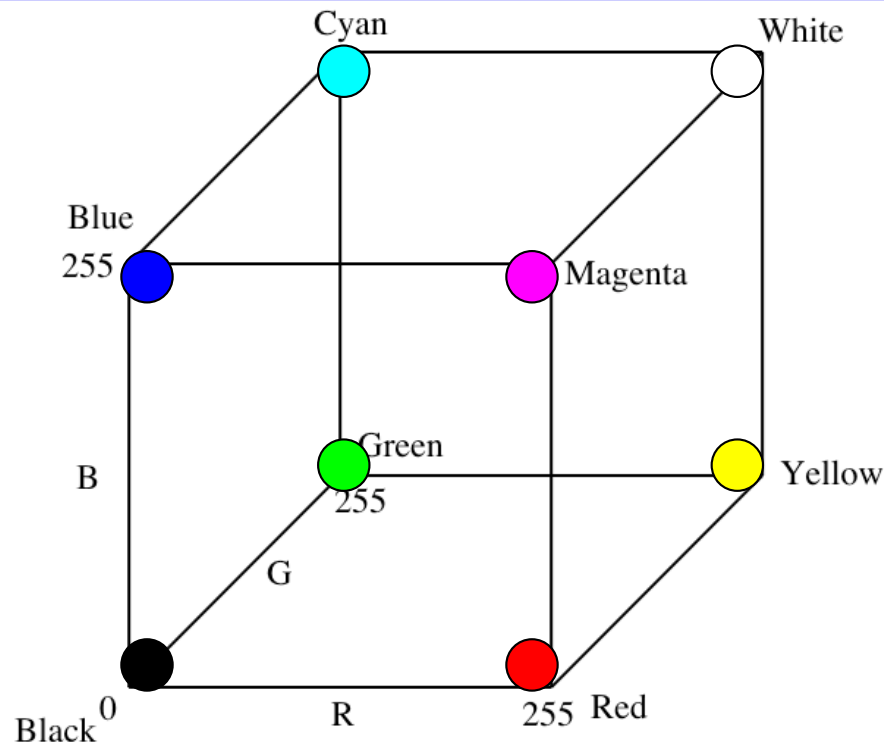
Repeat this *nAtom* times



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);
```



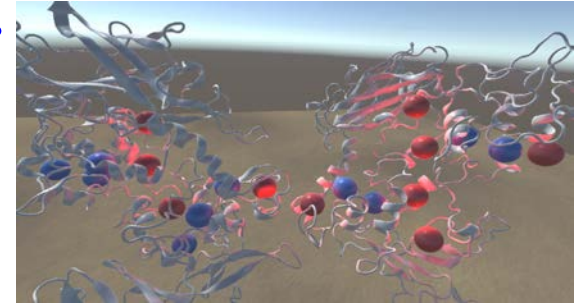
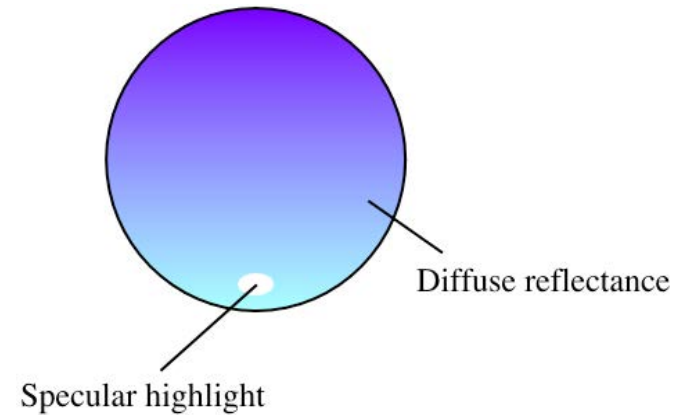
- **OpenGL as a state machine:** Color change stays.

Lighting & Materials

OpenGL color =
light \times material-reflectance

OpenGL Color Types

- **Diffuse component:** Gives the appearance of a matte 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

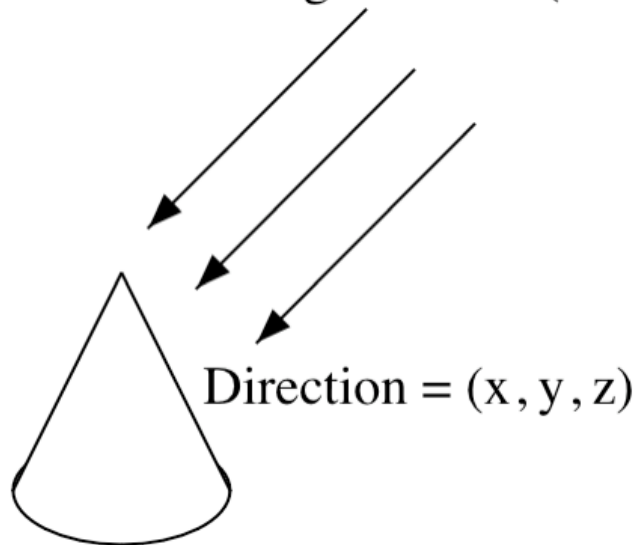
- **Refractance:** Material is characterized by ambient, diffuse & specular reflectance, *i.e.*, how the object reflects light.
- **glEnable(GL_COLOR_MATERIAL)**
In this mode, the current color specified by **glColor*()** will change the ambient & diffuse reflectance.

Lighting Source

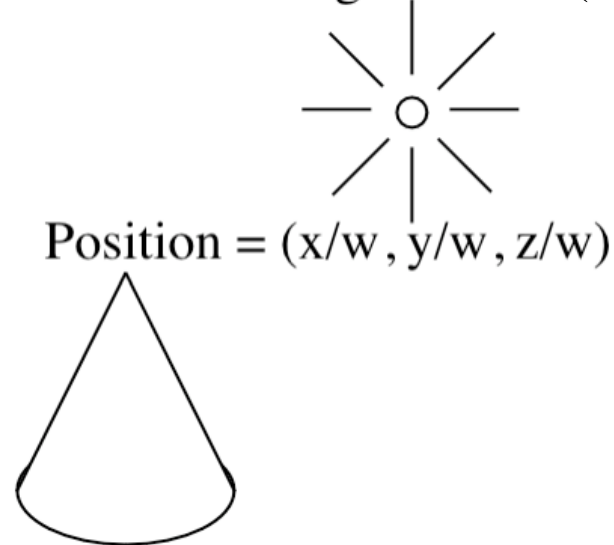
$\text{color} = \text{light} \times \text{material}$ (e.g., $\alpha = \alpha_{\text{light}} \times \alpha_{\text{material}}$)

```
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);
```

Directional light source ($w = 0$)



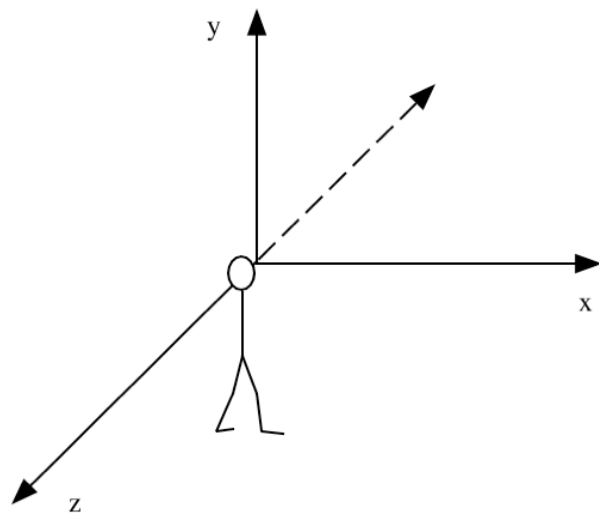
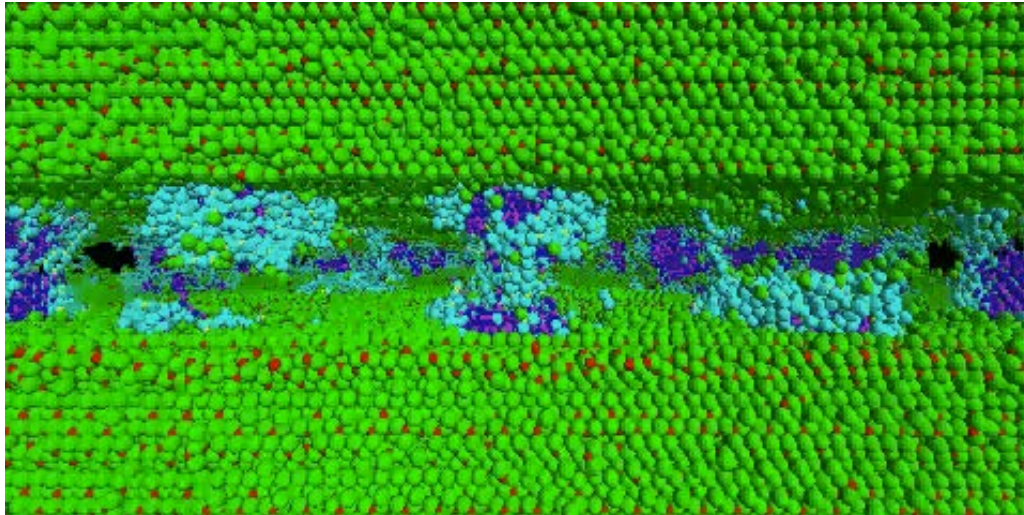
Point light source ($w \neq 0$)



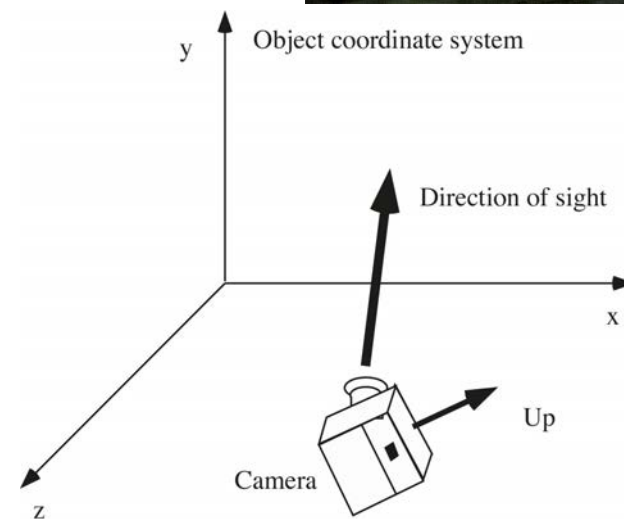
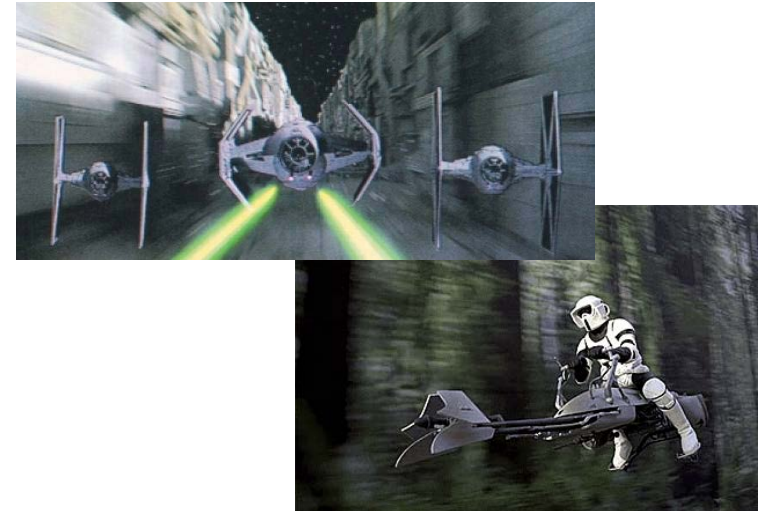
Viewing Transformation

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

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



Eye coordinate system



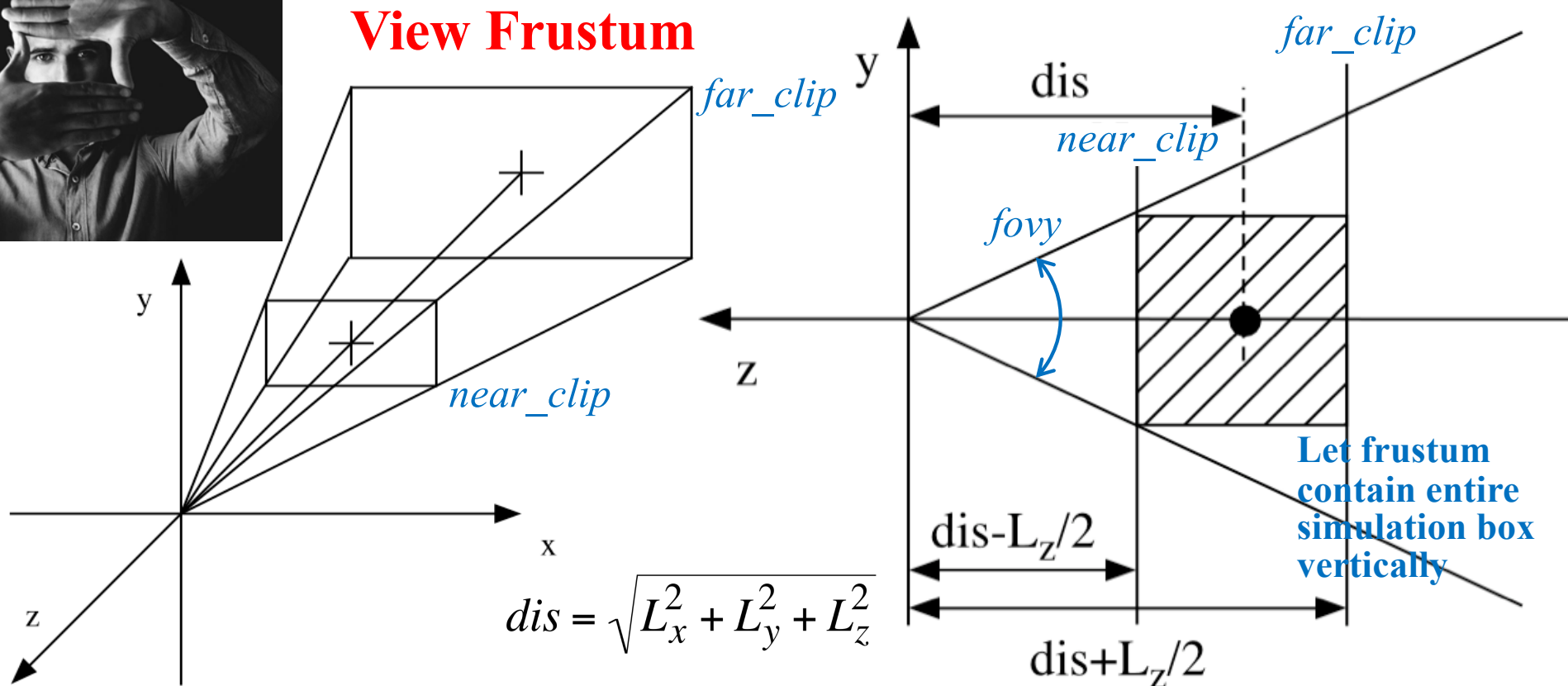
Camera specification

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);
}
```

$$fovy = 2 \tan^{-1}$$

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

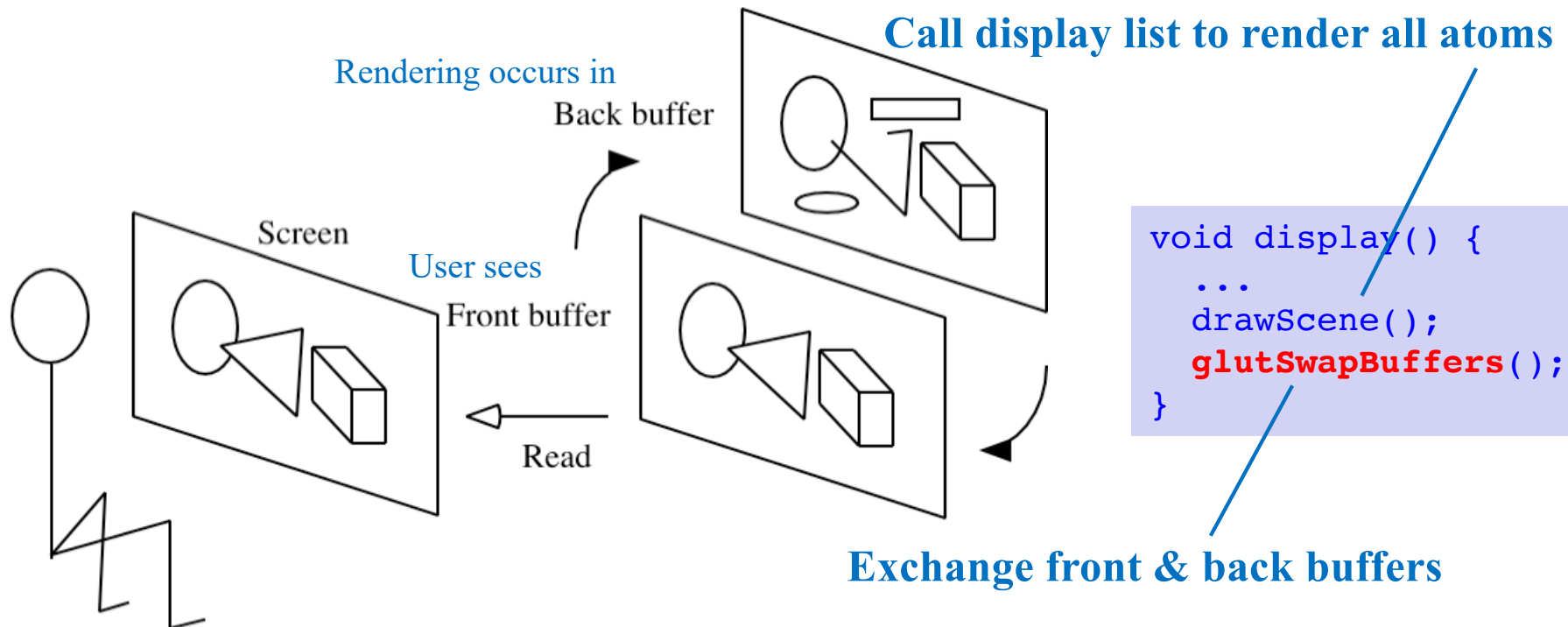


Animation

```
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 (make a display list) */  
        glutPostRedisplay();  
        ++stepCount;  
    }  
}
```

“idle” event handler: Called when current scene has been drawn & nothing to do

— Advance simulation one time-step



Do-It-Yourself MD Animation

- **Combine** `md.c` (<https://aiichironakano.github.io/cs596/src/md/>) & `atomv.c` (<https://aiichironakano.github.io/cs596/src/viz/>) **to write a C+OpenGL program for *in situ* animation of simulation, following the lecture note on “Visualizing Molecular Dynamics III—Animation”:**
<https://aiichironakano.github.io/cs596/Visual.pdf>

1. Initialize atomic coordinates, velocities, accelerations & step count before entering the GLUT main loop in `main()`
`InitParams(); // Read and initialize MD parameters`
`InitConf();`
`ComputeAccel(); // Compute initial accelerations`
`stepCount = 1; // Initialize the MD step count`
2. Register single-MD-step update function, say `animate()`, as `glutIdleFunc()` callback function
`glutIdleFunc(animate);`
3. In the callback function, `animate()`
`if stepCount ≤ StepLimit`
 - (i) velocity-Verlet integration for one MD step, `SingleStep()`;
 - (ii) make a display list for a collection of atoms with the updated atomic coordinates, *i.e.*, call `makeCurframeGeom()`;
 - (iii) call `glutPostRedisplay()` to redraw the updated scene;
 - (iv) increment the time step, `stepCount`;`endif`

Do-It-Yourself MD Animation (2)

4. Base program is atomv.c (it will be an OpenGL program)

Rename atomv.h|c to mdv.h|c

Copy (a) all contents of md.h into mdv.h & (b) all functions but main() from md.c to mdv.h; note most contents of main() in md.c have been used in animate() & main() in mdv.c in the previous slides

atomv.h	md.h
int natoms	int nAtom
AtomType *atoms	double r[NMAX][3]

Only used in makeAtoms() — replace by md.h counterparts

```
for (i=0; i < natoms; i++) {  
    glPushMatrix();  
    glTranslatef(atoms[i].crd[0],atoms[i].crd[1],atoms[i].crd[2]);  
    glColor3f(rval,gval,bval);  
    glCallList(sphereid);  
    glPopMatrix();  
}
```

makeAtoms() in atomv.c

```
for (i=0; i < nAtom; i++) {  
    glPushMatrix();  
    glTranslatef(r[i][0],r[i][1],r[i][2]);  
    glColor3f(rval,gval,bval);  
    glCallList(sphereid);  
    glPopMatrix();  
}
```

makeAtoms() in mdv.c