Visualizing Molecular Dynamics

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Goal: Visualize simulation to "understand" it

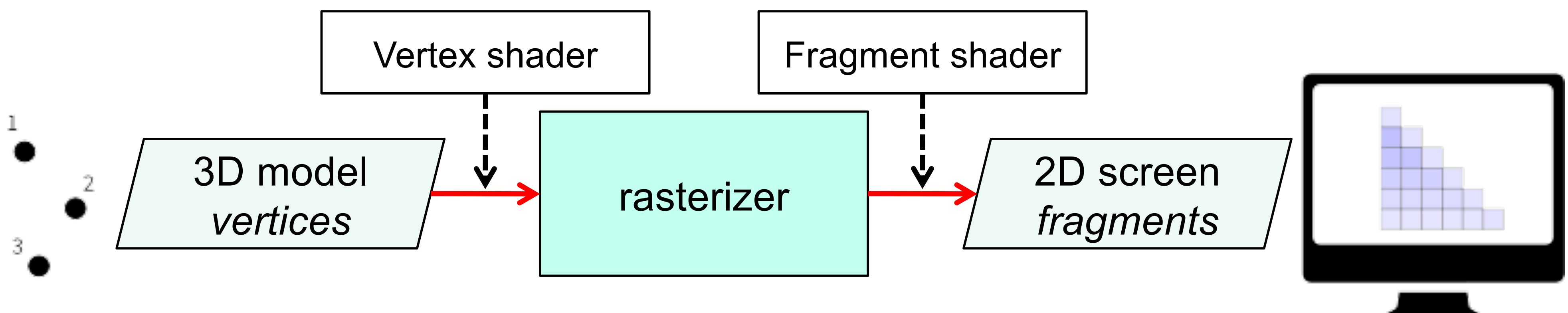
OpenGL: Getting Started

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

* **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)

⋮

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

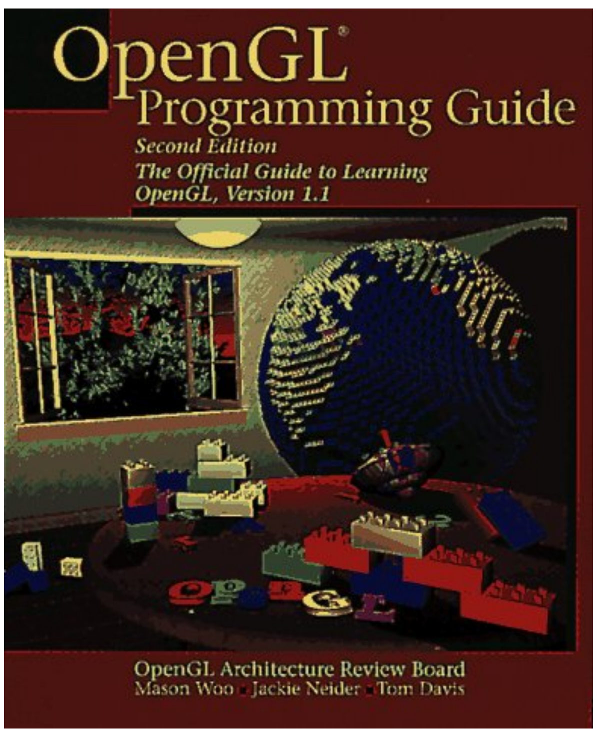
2008 OpenGL3.0: Major revision

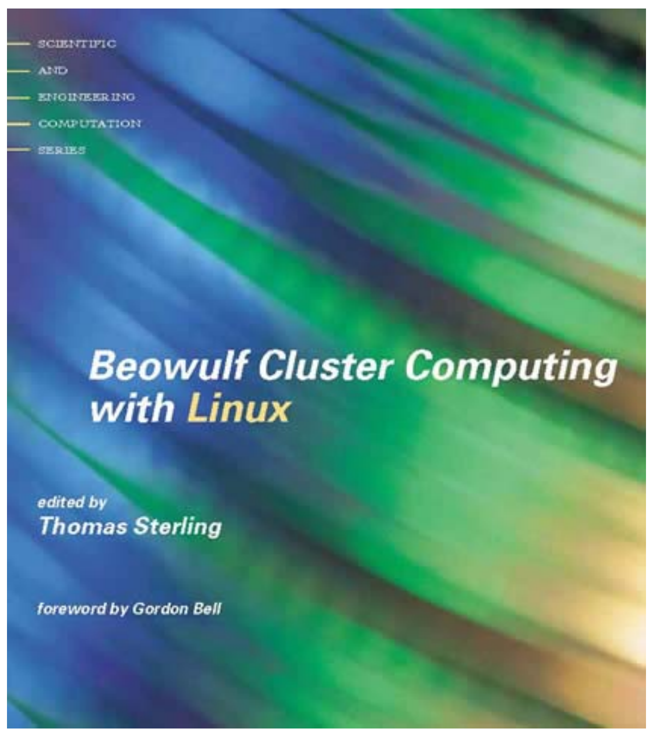
1994 Beowulf cluster computer
MPI 1.0 (message passing)
`MPI_Send(), MPI_Recv()`

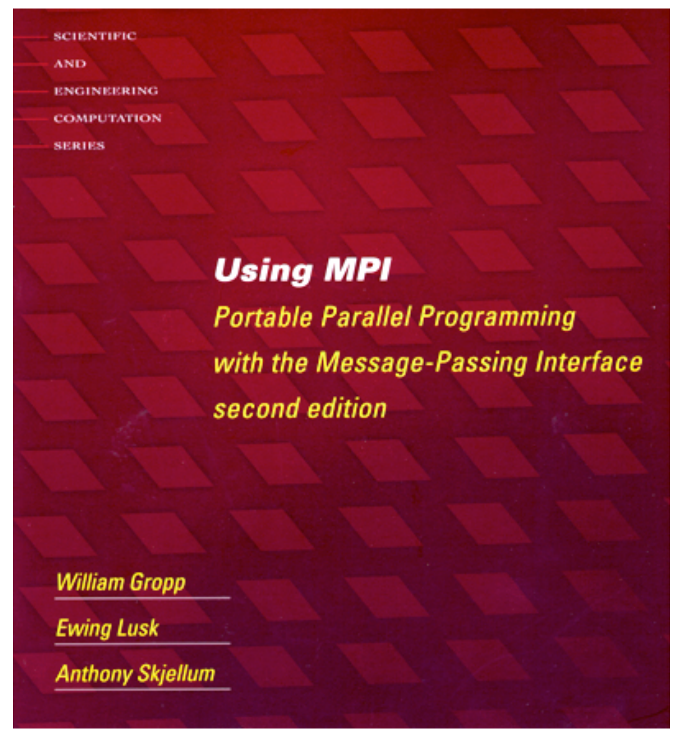
1997 OpenMP 1.0 (multithreading)
`#pragma omp parallel`

⋮

2007 CUDA 1.0 (graphics cards)





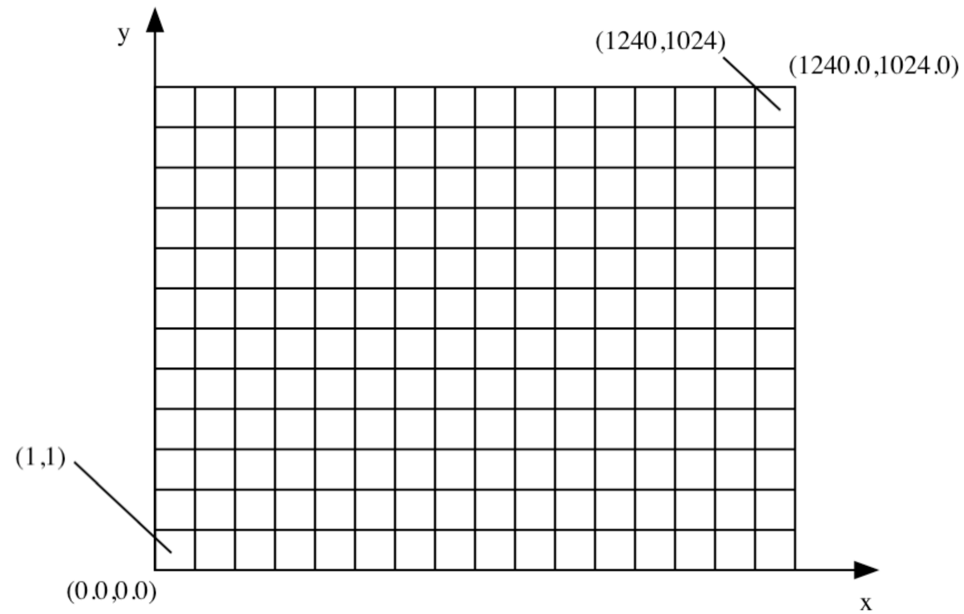


OpenGL Programming Basics

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);
  /* Start main display loop */
  glutMainLoop();
}

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

events

event handlers

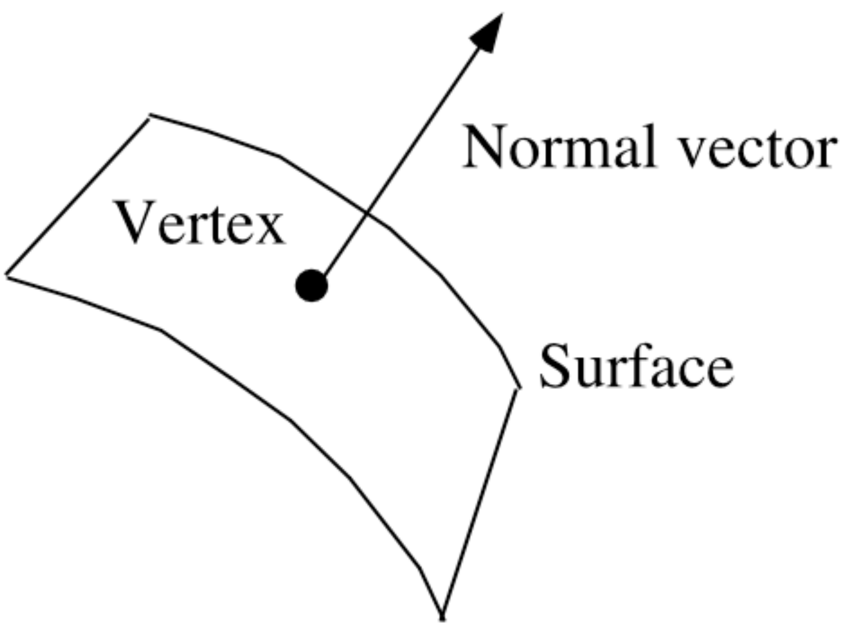
Glut runtime system keeps listening if any event happens; when an even happens, it invokes the corresponding user-specified event handler function.

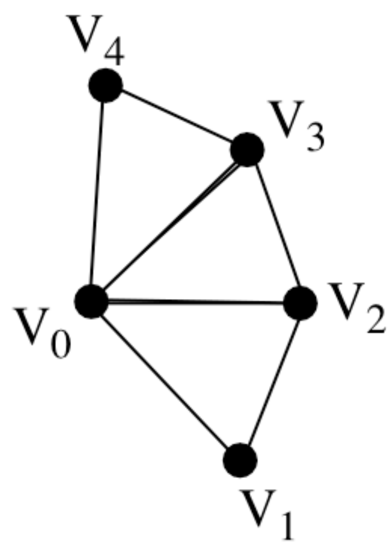
All topics in this presentation are detailed in
https://aiichironakano.github.io/cs596/Visual.pdf

Polygonal Surfaces

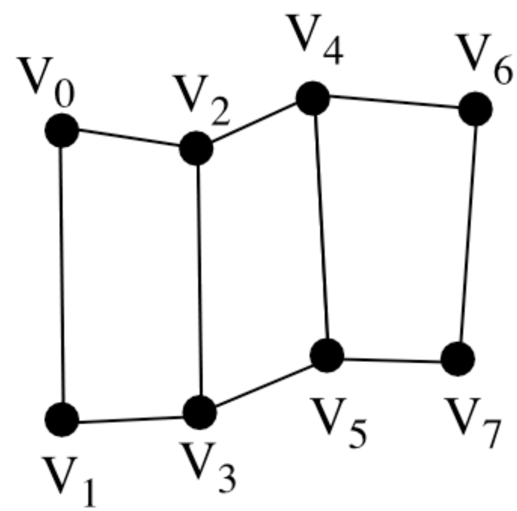
Drawing a set of polygons

```
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();
```





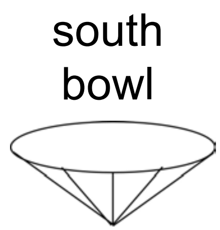
GL_TRIANGLE_FAN



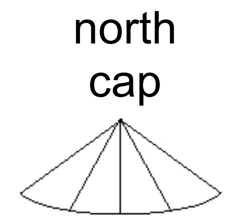
GL_QUAD_STRIP

Polygonal Sphere

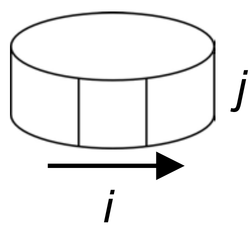
```
int nlon=18, nlat=9;
loninc = 2*M_PI/nlon; /* Δϕ */
latinc = M_PI/nlat;   /* Δθ */
/* South-pole triangular fan */
glBegin(GL_TRIANGLE_FAN);
  glNormal3f(0,-1,0);
  glVertex3f(0,-radius,0);
  lon = 0;
  lat = -M_PI/2 + latinc;
  y = sin(lat);
  for (i=0; i<=nlon; i++) {
    x = cos(lon)*cos(lat);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



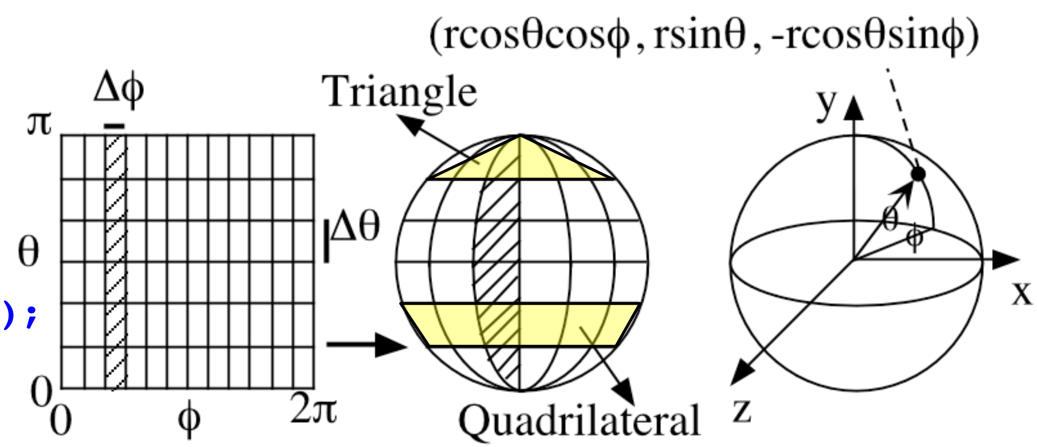

```
/* North-pole triangular fan */
glBegin(GL_TRIANGLE_FAN);
  glNormal3f(0,1,0);
  glVertex3f(0,radius,0);
  y = sin(lat);
  lon = 0;
  for (i=0; i<=nlon; i++) {
    x = cos(lon)*cos(lat);
    z = -sin(lon)*cos(lat);
    glNormal3f(x,y,z);
    glVertex3f(x*radius,y*radius,z*radius);
    lon += loninc;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




```
/* 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 → 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(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.

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

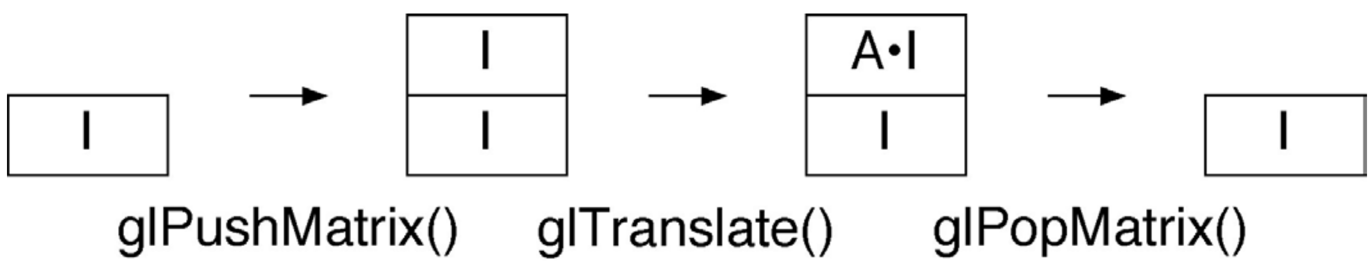
$$\begin{bmatrix} x' \\ y' \\ z' \\ 1 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix}$$

```
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();
```

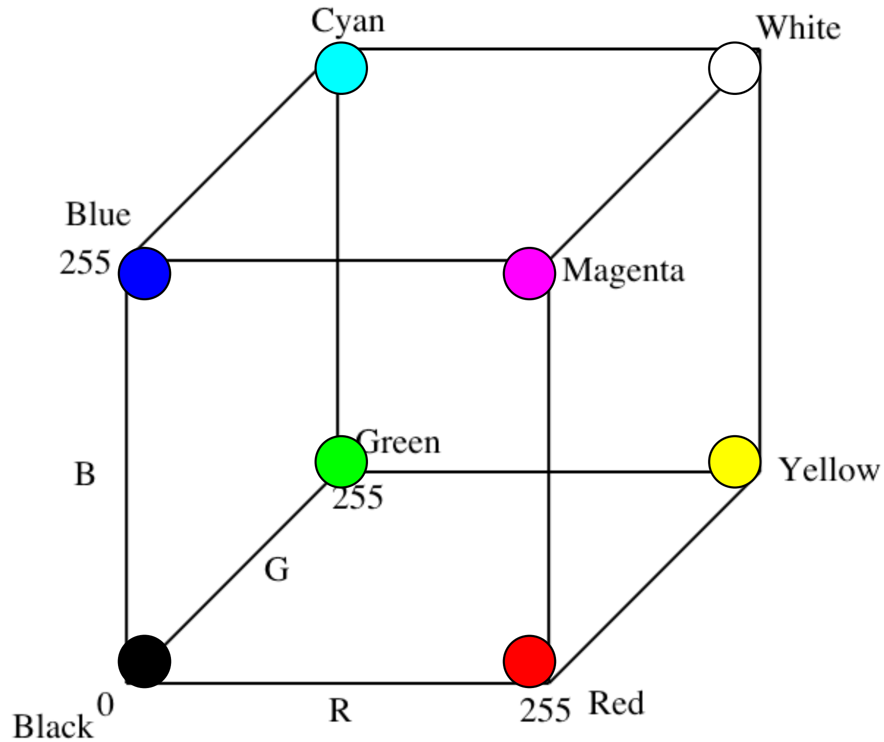
Repeat this *nAtom* times



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.

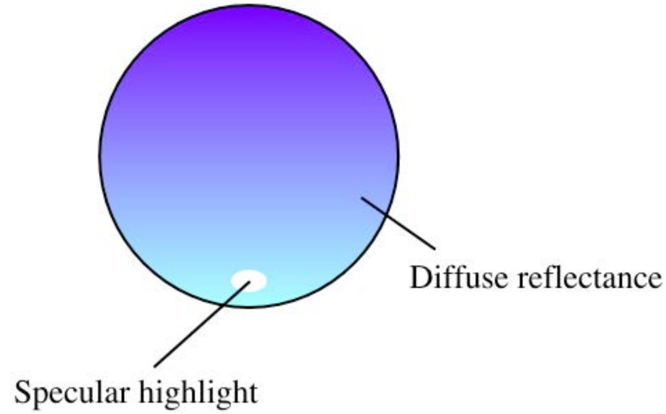
```
float r=1.0, g=0.0, b=0.0;

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



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

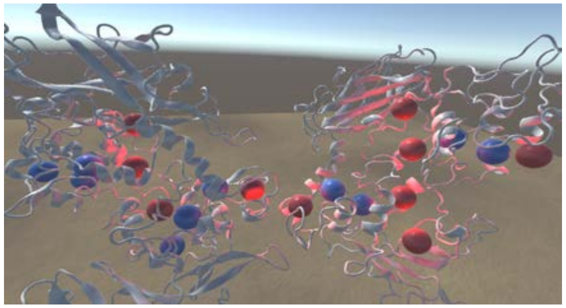
Lighting & Materials

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.



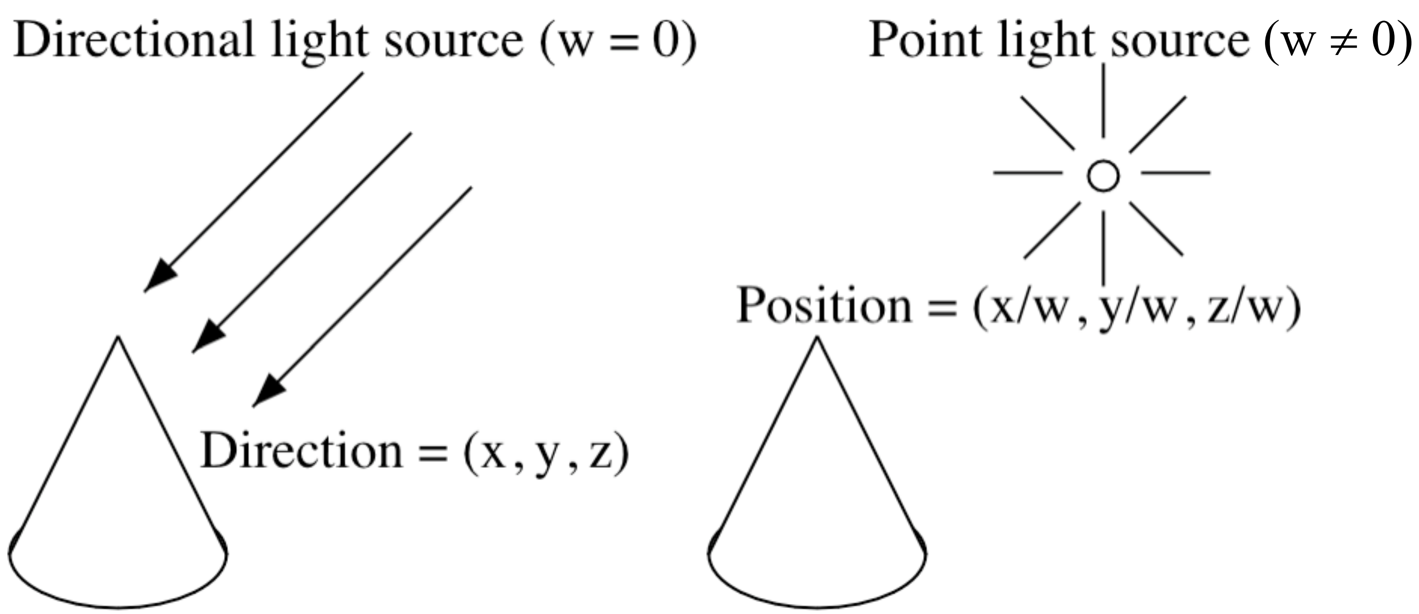
Materials Definition

- **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.*, $\alpha = \alpha_{light} \times \alpha_{material}$)

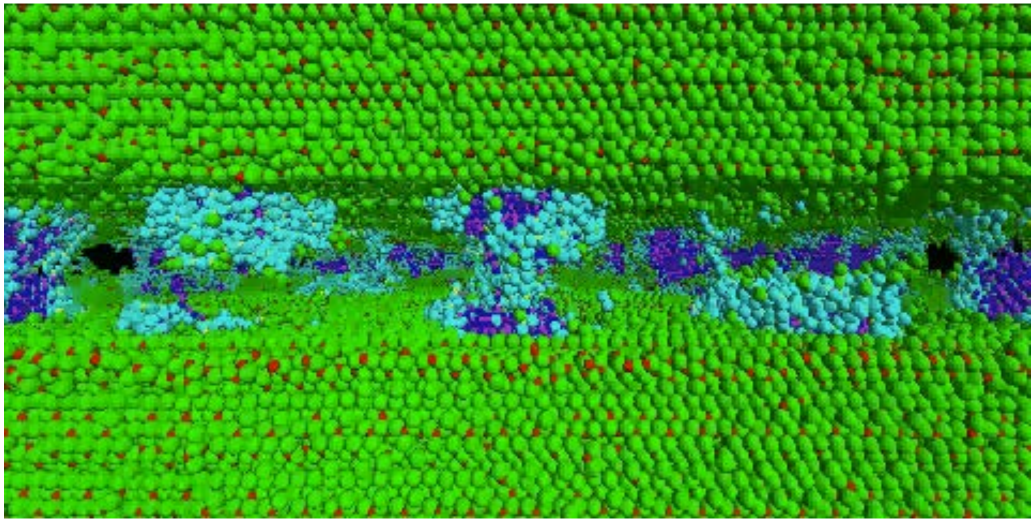
```
float light_diffuse[4] = {1.0,1.0,1.0,1.0};
float light_position[4] = {0.5,0.5,1.0,0.0};

/* 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);
```

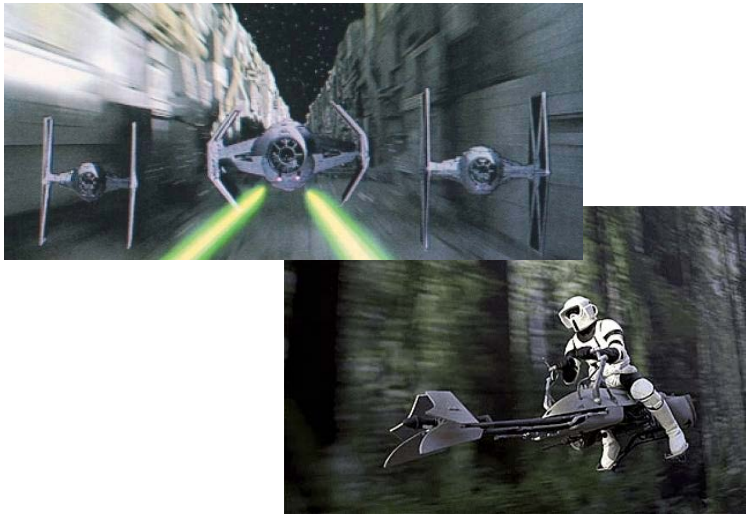


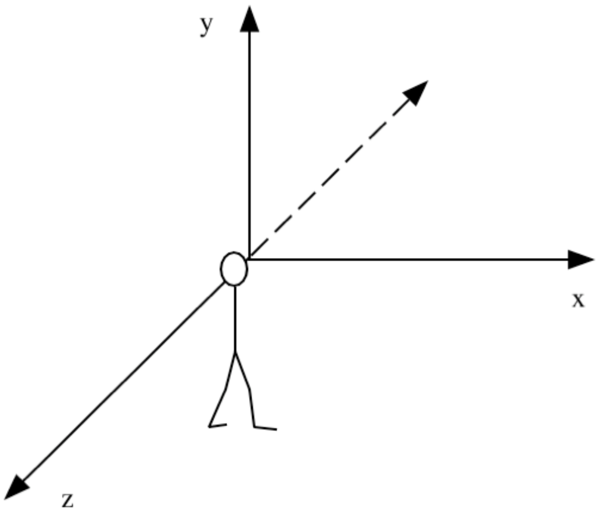
Viewing Transformation

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

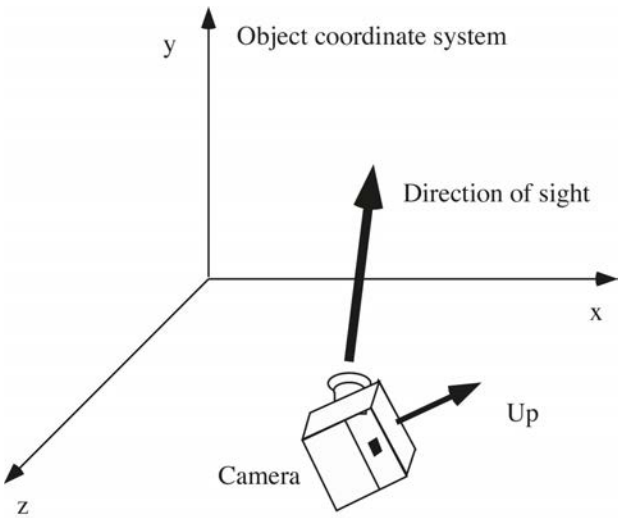
```
gluLookat(eyx, eyey, eyz, centerx, centery, centerz, upx, upy, upz);
```







Eye coordinate system



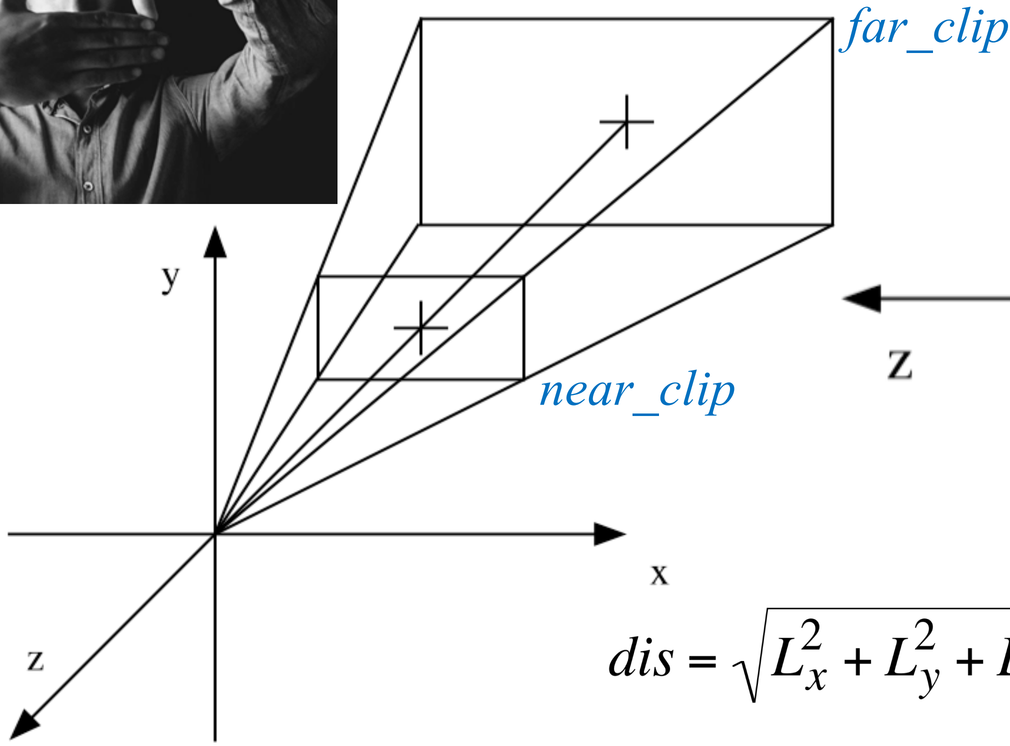
Camera specification

Clipping

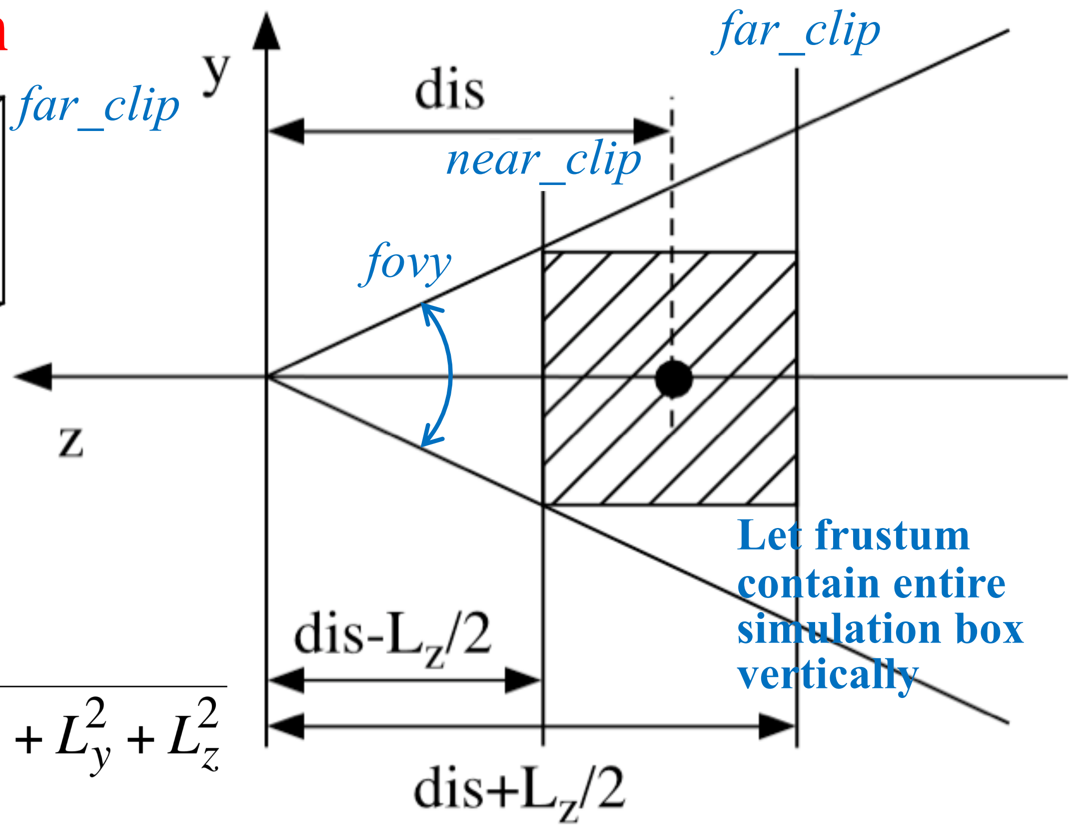
```
void reshape (int w, int h) {
  ...
  /* set the GL viewport to match the full size of the window */
  glViewport(0, 0, (GLsizei)w, (GLsizei)h);
  aspect = w/(float)h;
  glMatrixMode(GL_PROJECTION);
  glLoadIdentity();
  gluPerspective(fovy,aspect,near_clip,far_clip);
  glMatrixMode(GL_MODELVIEW);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

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

View Frustum



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



Animation

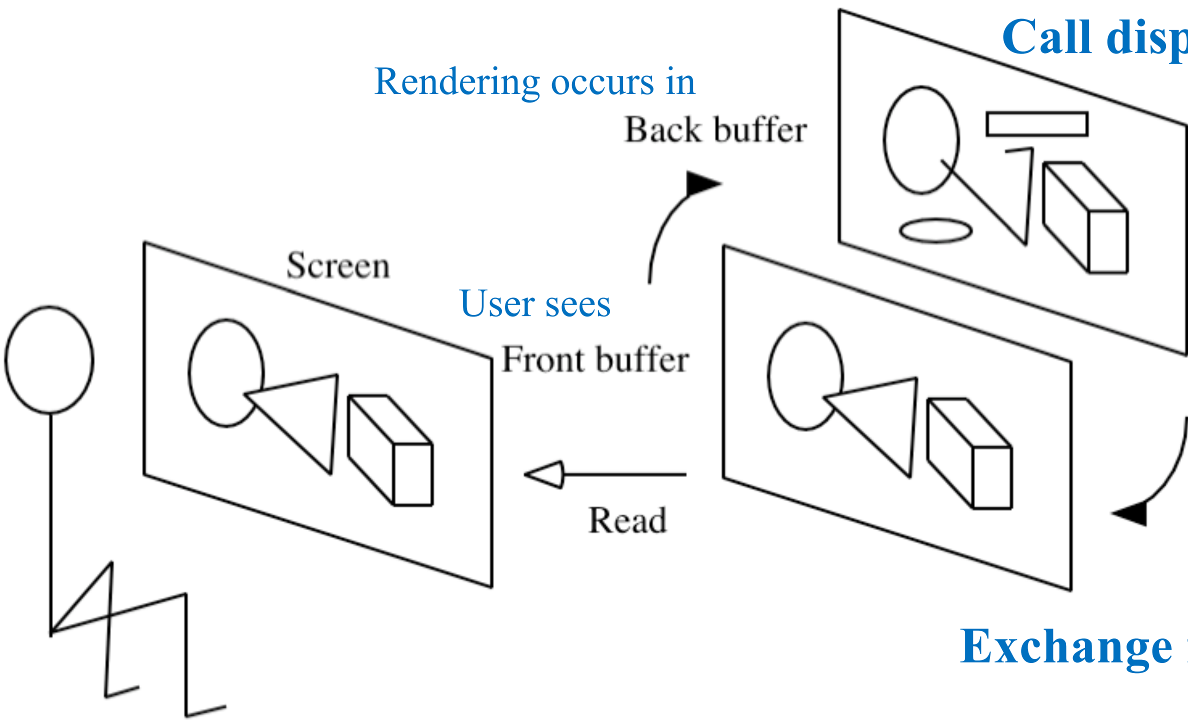
```
main() {
  glutIdleFunc(animate);
}
```

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

Advance simulation one time-step

```
...
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;
  }
}
```

glutPostRedisplay(): Force display event ~ user request for display() call



Call display list to render all atoms

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

Exchange front & back buffers

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 atomv.h & (b) all functions but main() from md.c to atomv.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

makeAtoms() in atomv.c

```
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 mdv.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();
}
```