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complex nano materials: the chair of materials science and nanotechnology

Raytracing and atomistic rendering

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Nanoseminar, Dresden, 28. 07. 2011

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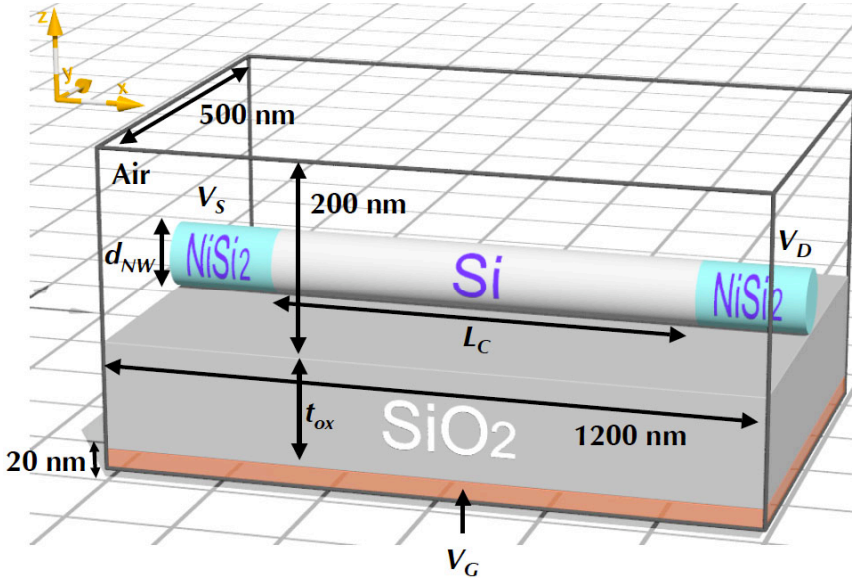
Preface

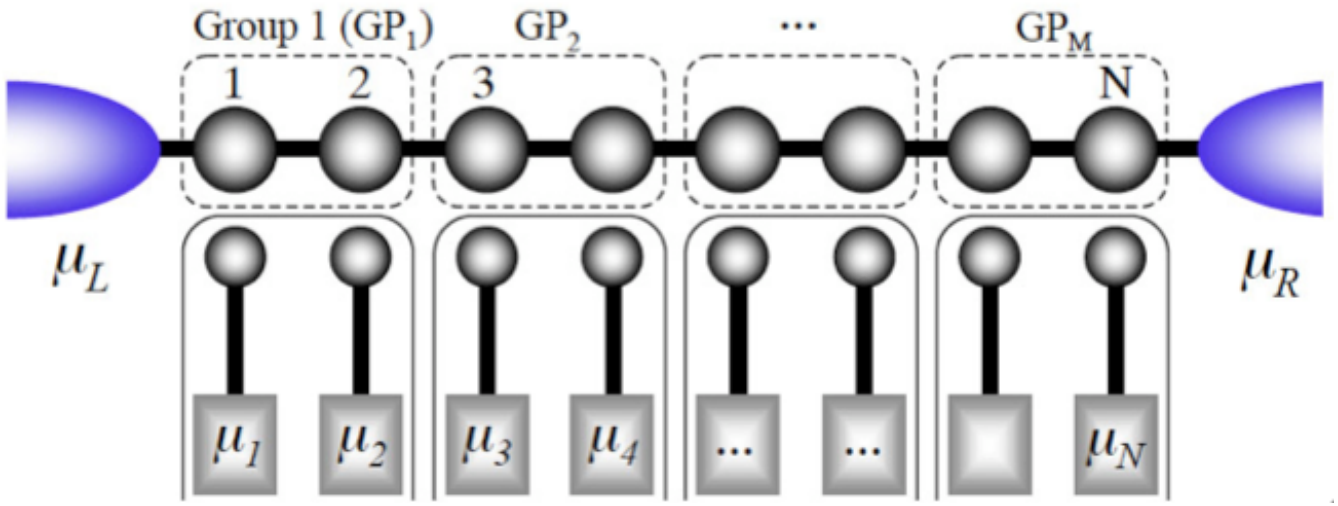
When people read a paper, they will look it on the following order;

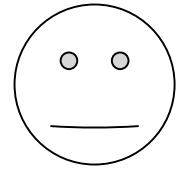
(1) Title
(2) Figures
(3) Abstract
(4) Conclusion
(5) Introduction …



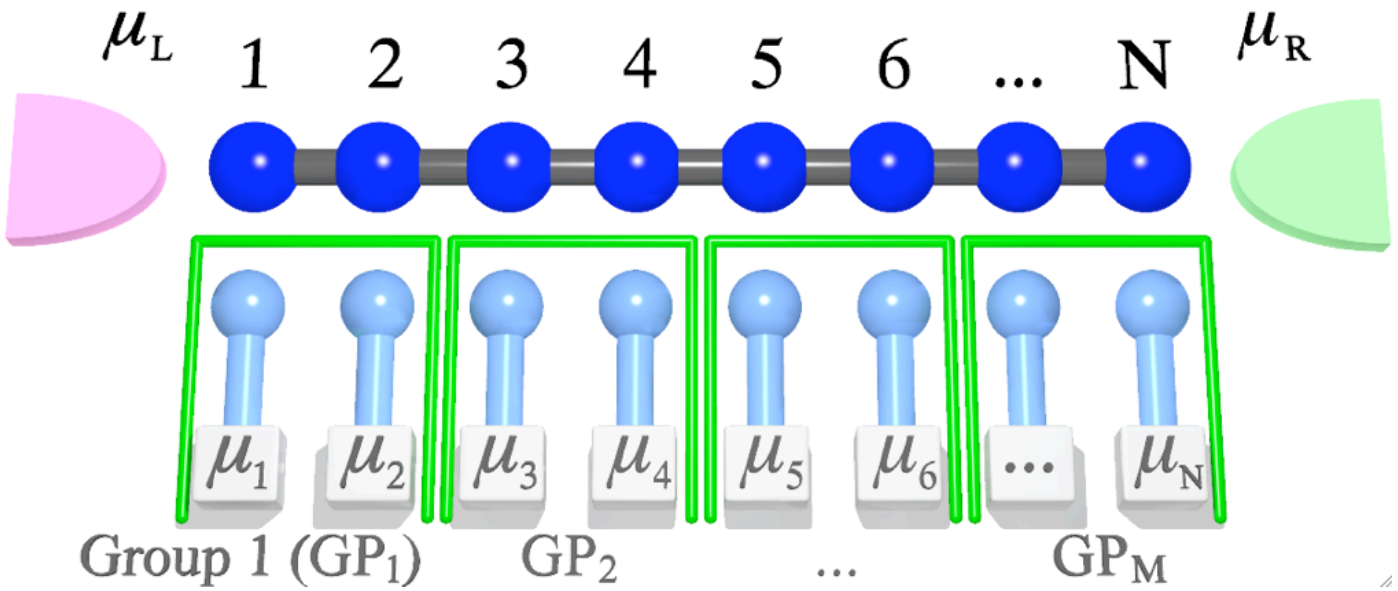
Making nice-looking or eye-catching figures are important for attracting the attention of audience.

Before





After



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Povray

There are many benefit to use Povray for raytracing.

Povray is one of the most famous application for reytracing

(1) Free
(2) For Windows, Mac, Linux
(3) Many web sites and tutorials
(4) It’s like Latex, code & render
(5) Several modelers available

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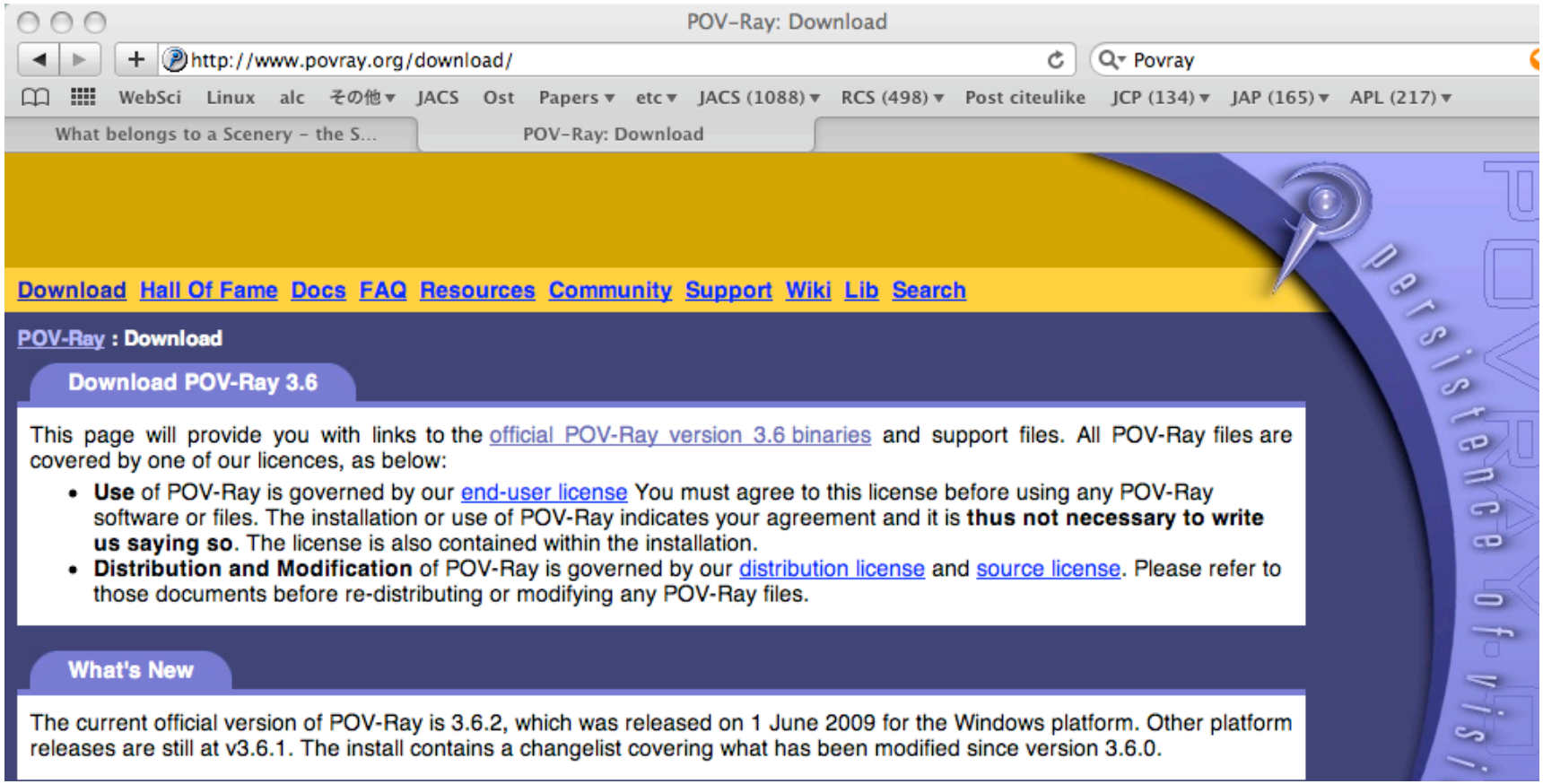
Installation of Povray

1. Go to official website http://www.povray.org/
2. Download binary http://www.povray.org/download/



In our institute povray for Linux is preinstalled, but it is CUI.

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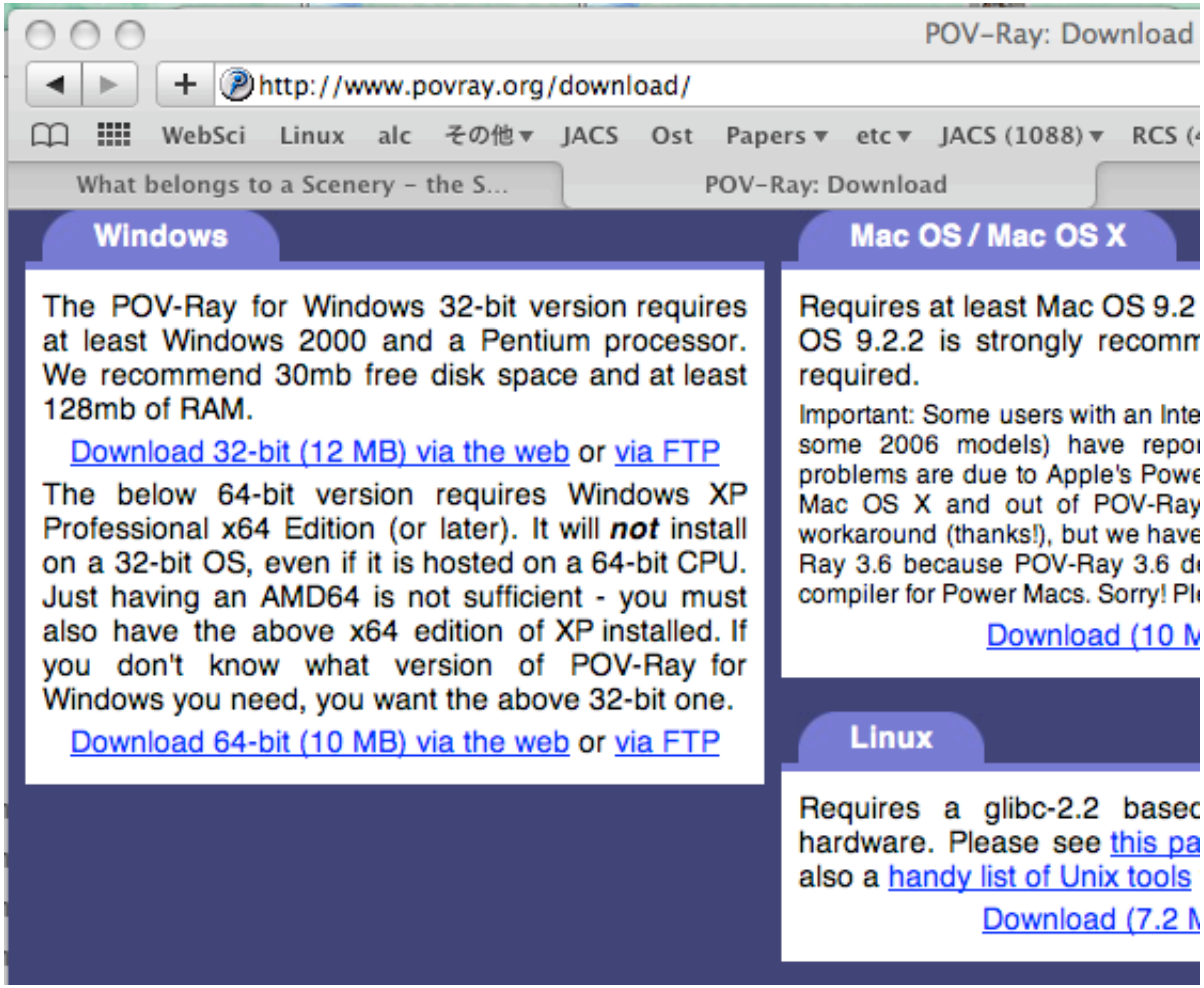
Installation of Povray

1. Go to official website http://www.povray.org/
2. Download binary http://www.povray.org/download/



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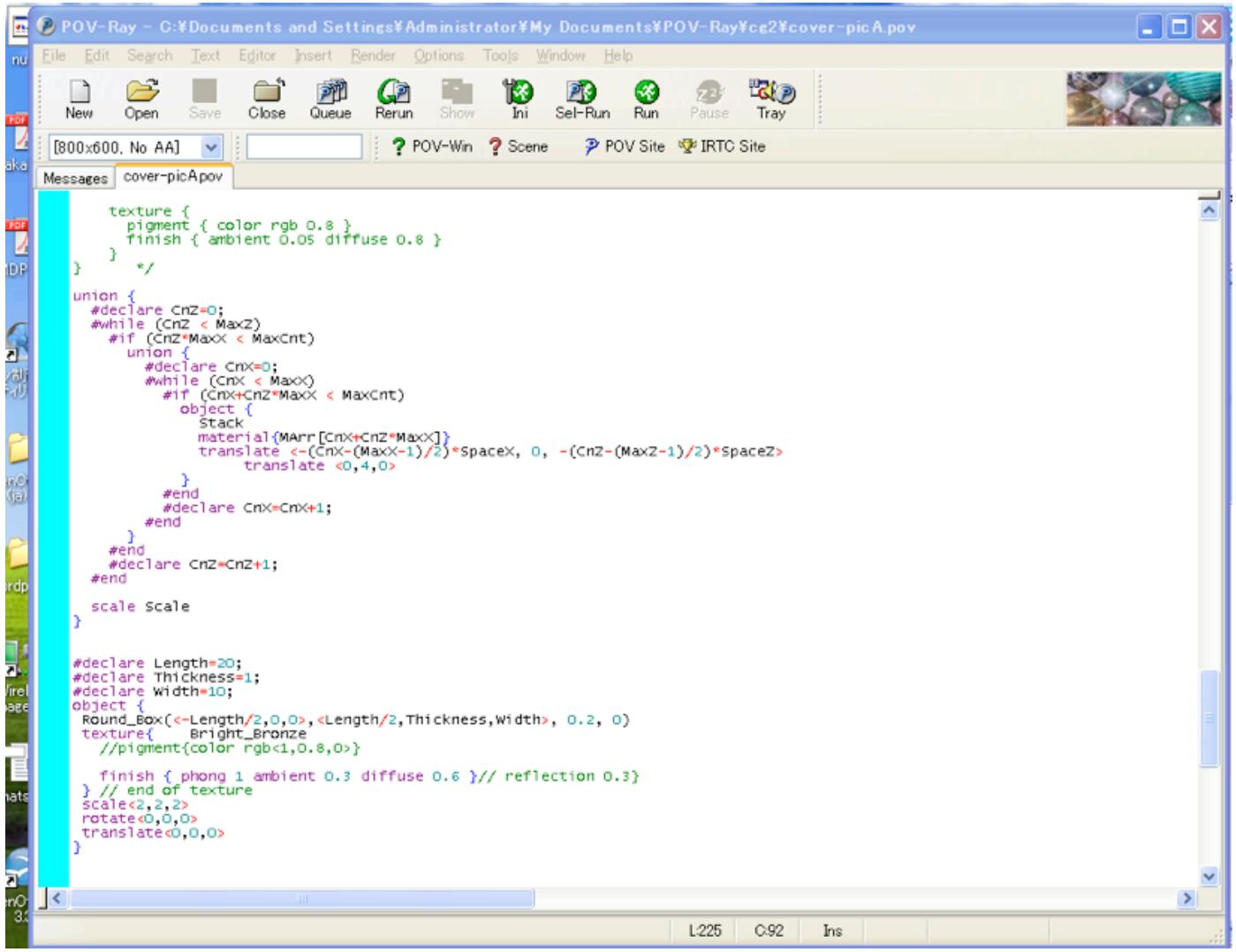
Interface of Povray

This is Povray version 3.6 in Windows.



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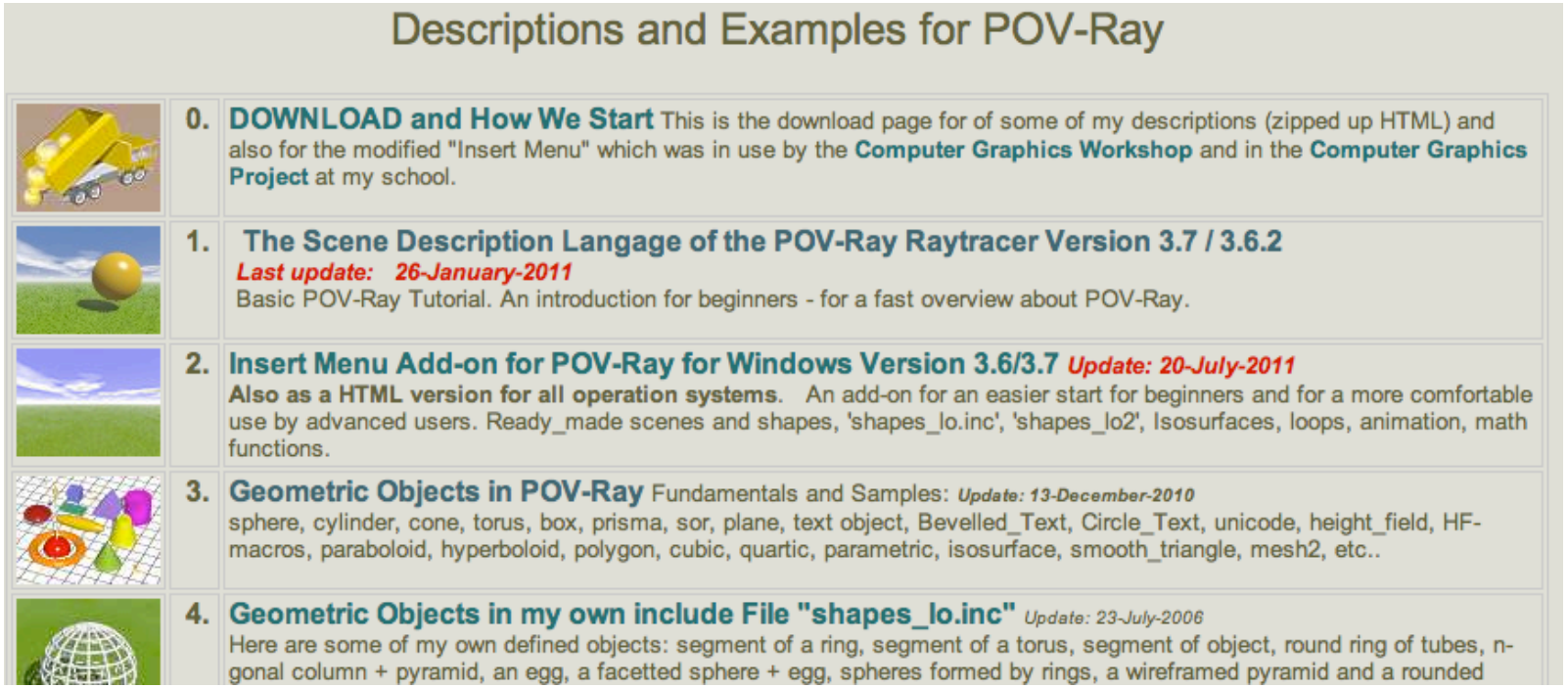
Best website

1. Search “Lohmueller povray” on Google
2. Nice tutorials
3. Many examples, templates, and explanations
4. Written in English, German, Italian, and French
5. He also provides extremely useful macro



Descriptions and Examples for POV-Ray

0. **DOWNLOAD and How We Start** This is the download page for of some of my descriptions (zipped up HTML) and also for the modified "Insert Menu" which was in use by the **Computer Graphics Workshop** and in the **Computer Graphics Project** at my school.

1. **The Scene Description Langage of the POV-Ray Raytracer Version 3.7 / 3.6.2**
Last update: 26-January-2011
Basic POV-Ray Tutorial. An introduction for beginners - for a fast overview about POV-Ray.

2. **Insert Menu Add-on for POV-Ray for Windows Version 3.6/3.7** *Update: 20-July-2011*
Also as a HTML version for all operation systems. An add-on for an easier start for beginners and for a more comfortable use by advanced users. Ready_made scenes and shapes, 'shapes_lo.inc', 'shapes_lo2', Isosurfaces, loops, animation, math functions.

3. **Geometric Objects in POV-Ray** Fundamentals and Samples: *Update: 13-December-2010*
sphere, cylinder, cone, torus, box, prisma, sor, plane, text object, Bevelled_Text, Circle_Text, unicode, height_field, HF-macros, paraboloid, hyperboloid, polygon, cubic, quartic, parametric, isosurface, smooth_triangle, mesh2, etc..

4. **Geometric Objects in my own include File "shapes_lo.inc"** *Update: 23-July-2006*
Here are some of my own defined objects: segment of a ring, segment of a torus, segment of object, round ring of tubes, n-gonal column + pyramid, an egg, a facetted sphere + egg, spheres formed by rings, a wireframed pyramid and a rounded

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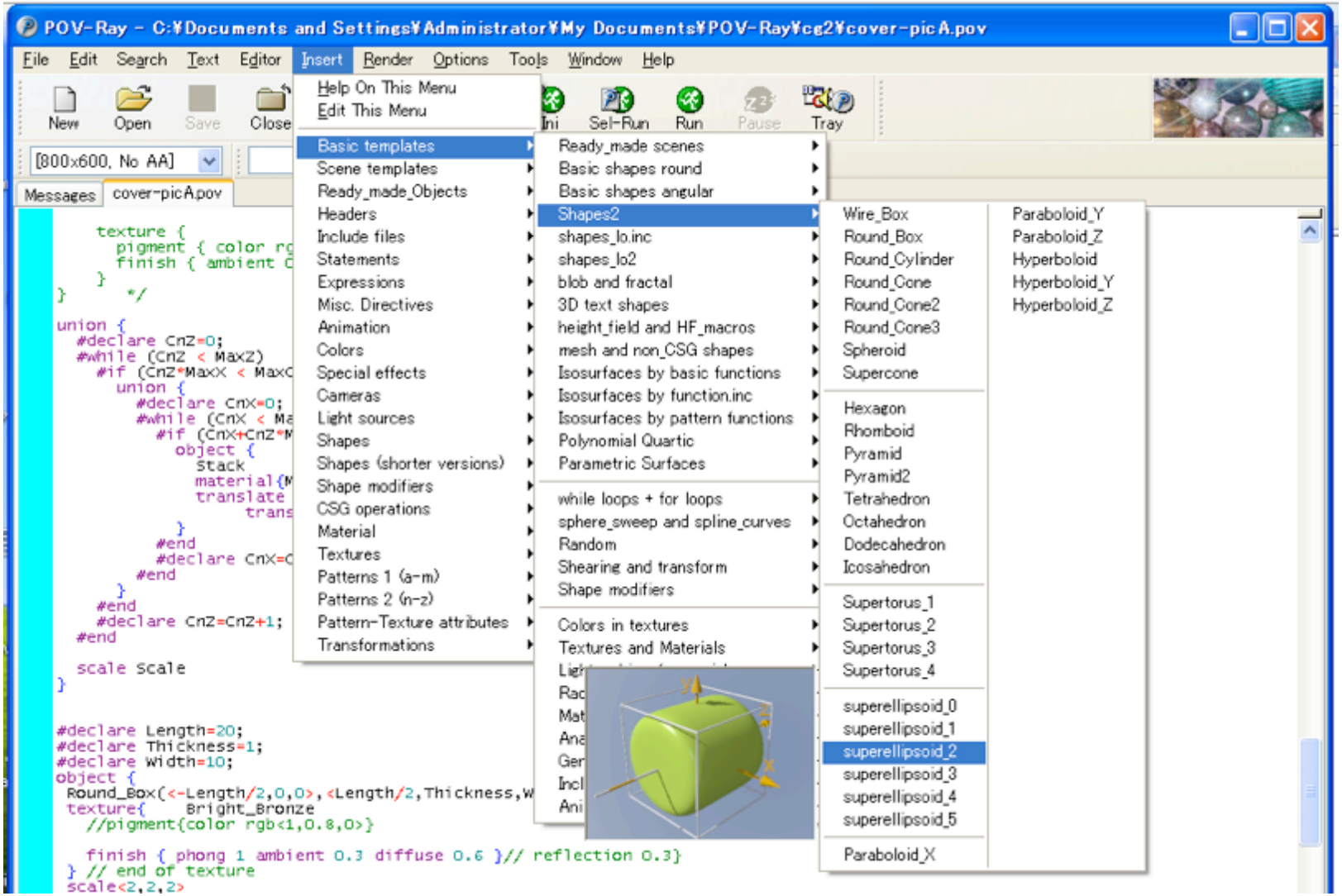
Best website

He also provides extremely useful macro



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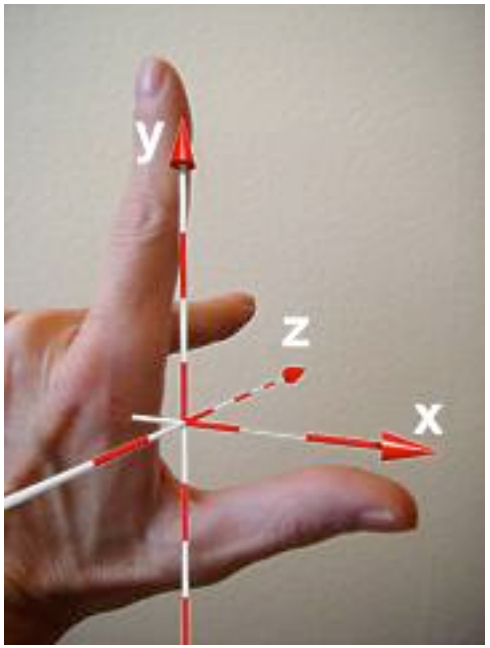
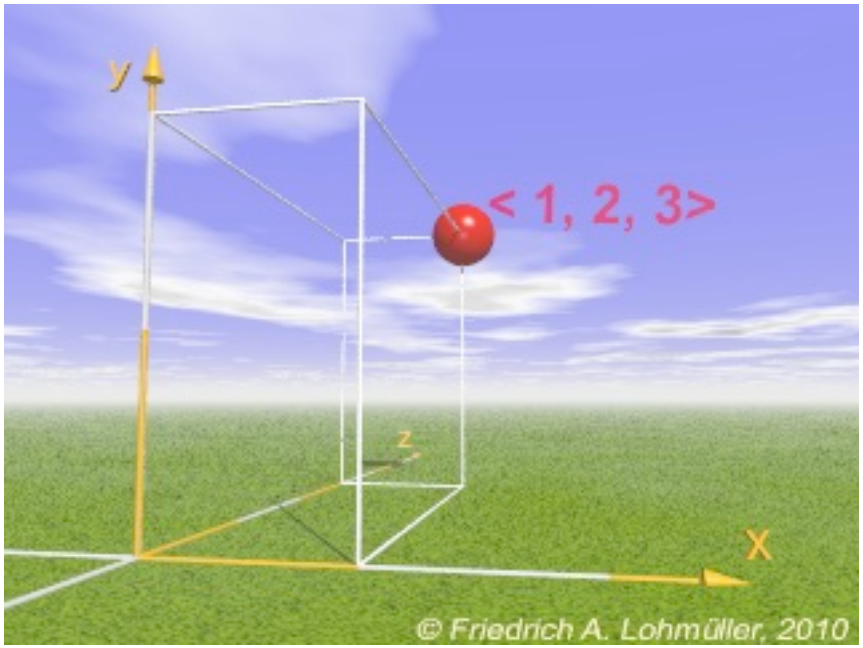
3D Global coordinate

For right handed people, you can code with checking the coordinate.





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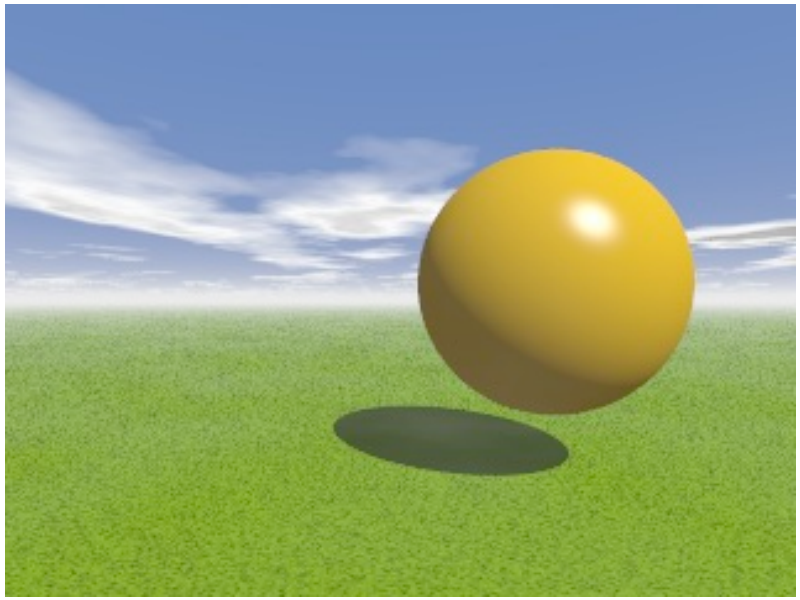
Procedures for modeling scenes

Here I show major procedures for making a scene.

(1) Set the position of camera
(2) Set the direction of camera
(3) Set the position of **light source**
(4) Set the **sky**
(5) Make the **floor**
(6) Put the **sphere**
(7) Set the properties of each **component**



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The simplest sample (sample.pov)

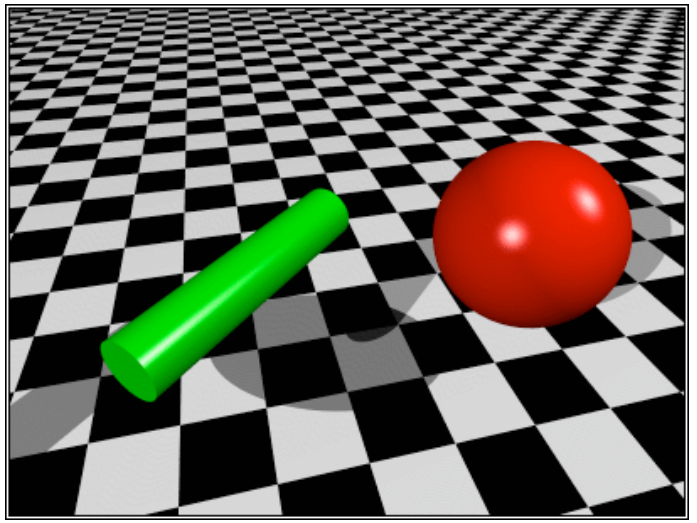
```
#include "colors.inc"
camera {  location  <-3, 4, -2>
          look_at   <-2, 1,  2>
}

light_source {    <-30, 20, -20> color White}
light_source {    <30, 30, -10> color White}

sphere {    <0, 1, 2> 1
   pigment { color Red }
   finish  { phong 0.8 }
}

cylinder {    <-4, 1, 1> <-2, 1, 3>, 0.3
   pigment { color rgb<0.0, 1.0, 0.0> }
   finish  { phong 0.8 }
}

plane {    <0, 1, 0>, -1
   pigment {          checker color Black color White    }
}
```



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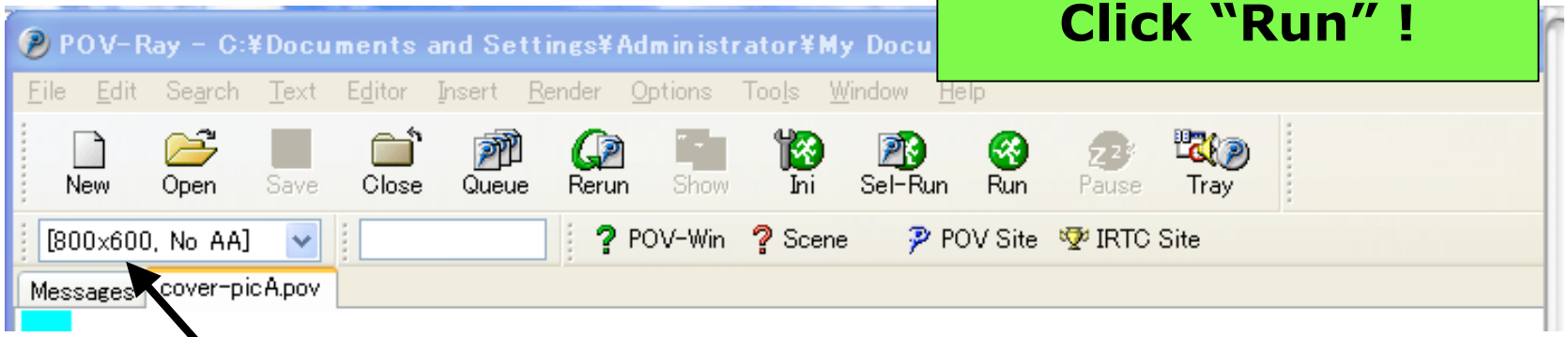
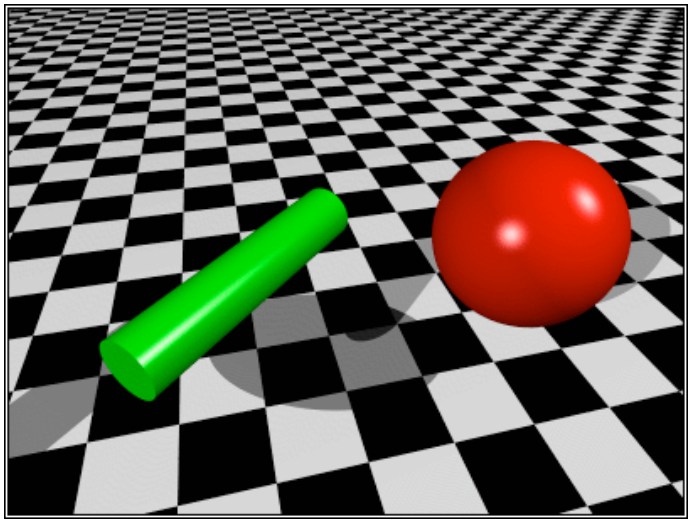
The simplest sample (sample.pov)



Click "Run" !

Size of image

You will get the image!



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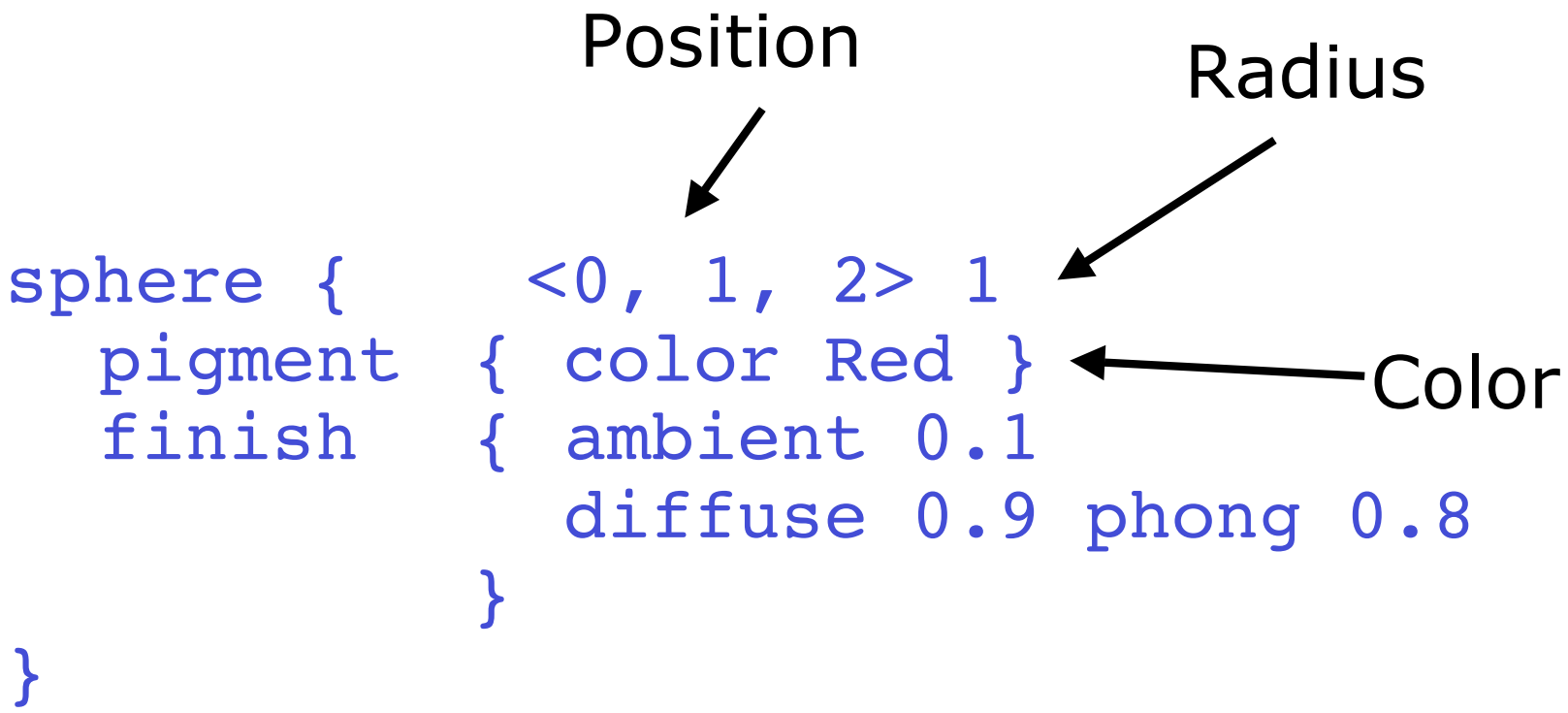
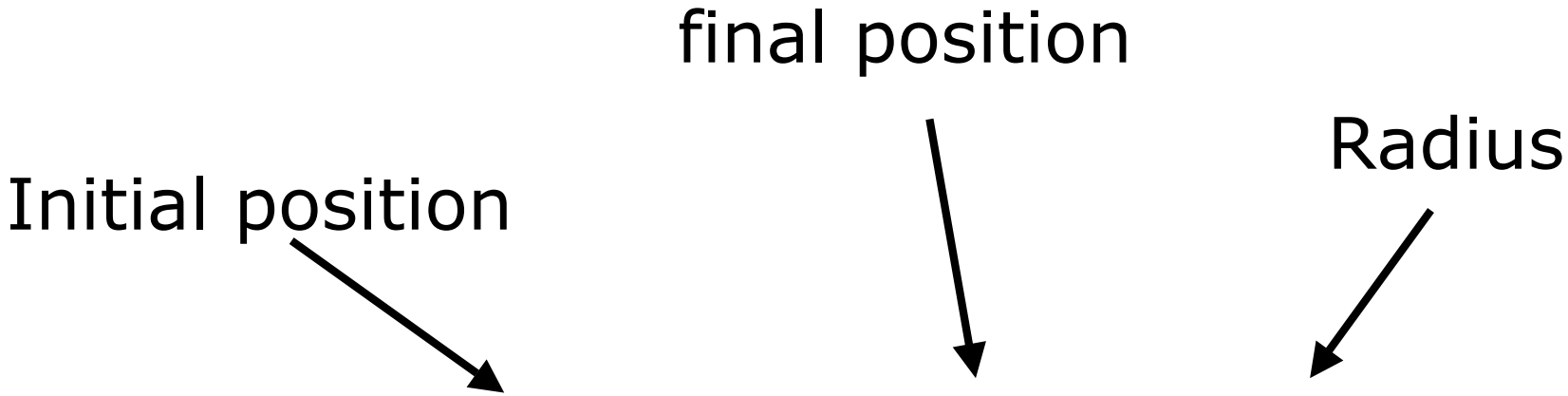
Sphere



Cylinder




```
cylinder {     <-4, 1, 1> <-2, 1, 3>, 0.3
   pigment { color rgb<0.0, 1.0, 0.0> }
   finish  { ambient 0.1 diffuse 0.9 phong 0.8 }
}
```

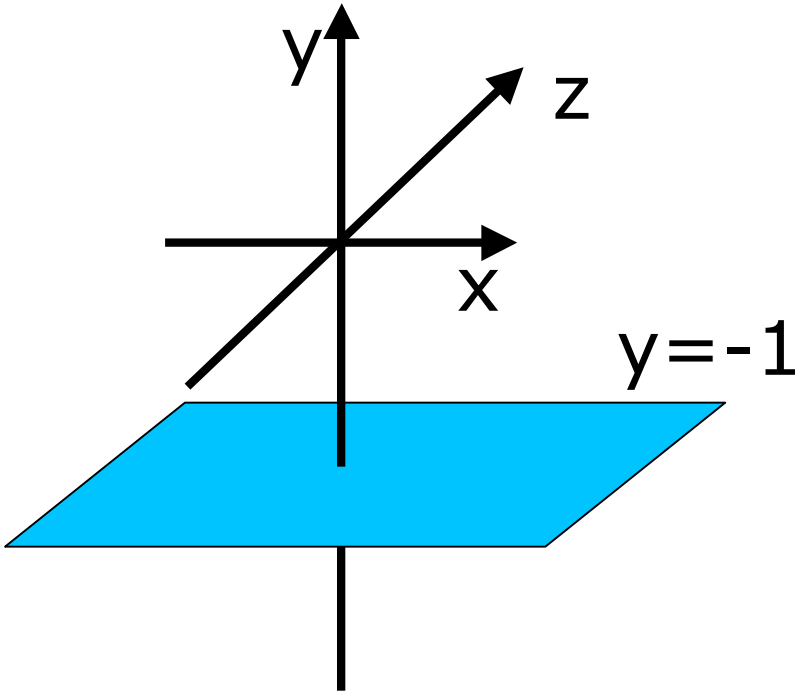
Floor

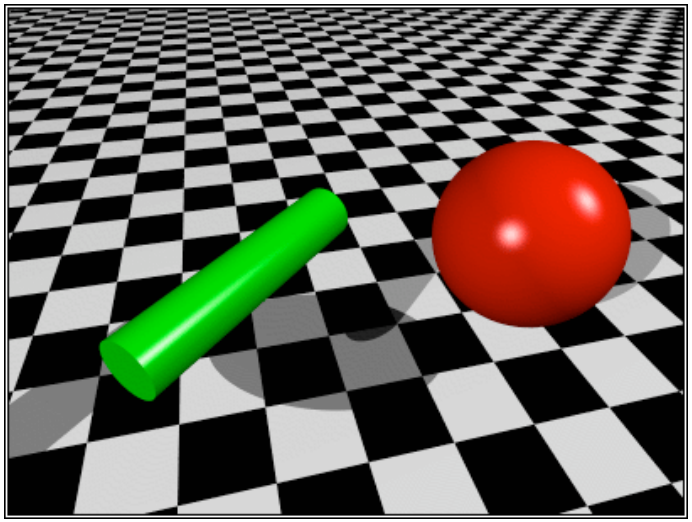
Normal vector

This means (y = -1)

Radius

```
plane {     <0, 1, 0>, -1
    pigment {          checker color Black color White    }
}
```





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Finish command

"finish" command sets the properties of the surface of primitive objects

```
sphere {     <0, 1, 2> 1
  pigment{ color Red }
  finish { ambient 0.1 diffuse 0.9 phong 0.8 }
}
```

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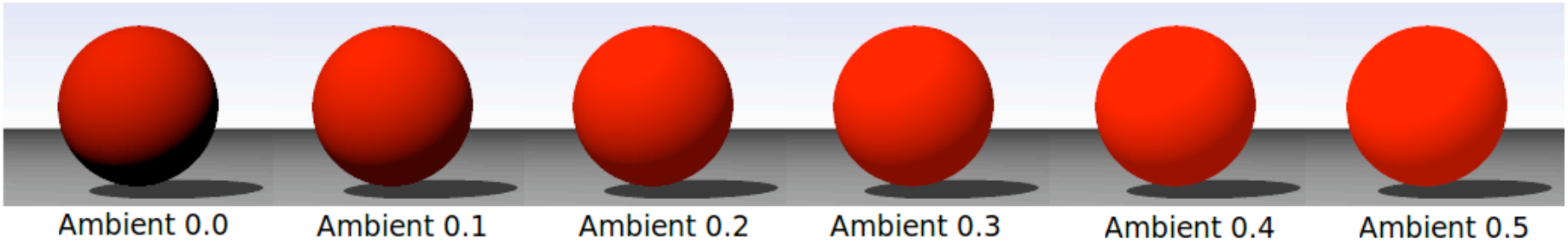
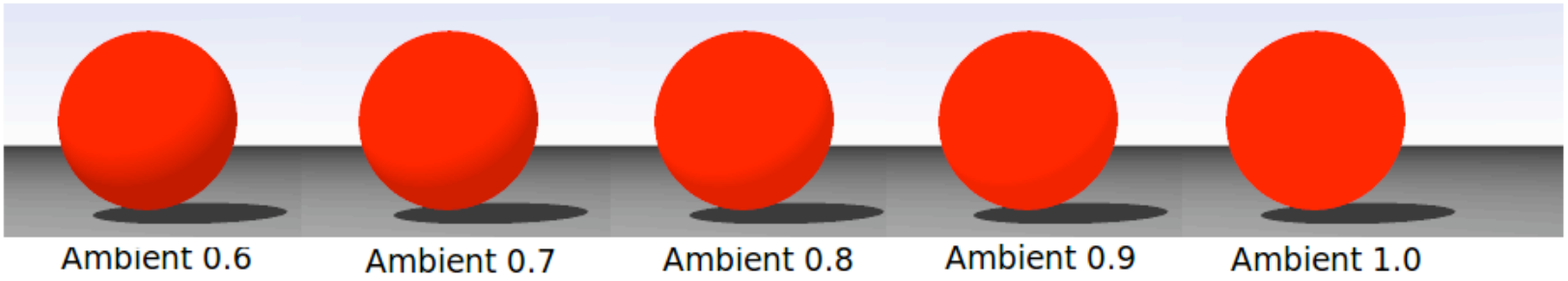
Ambient property

```
sphere {     <0, 1, 2> 1
  pigment{ color Red }
  finish { ambient 0.1 diffuse 0.9 phong 0.8 }
}
```





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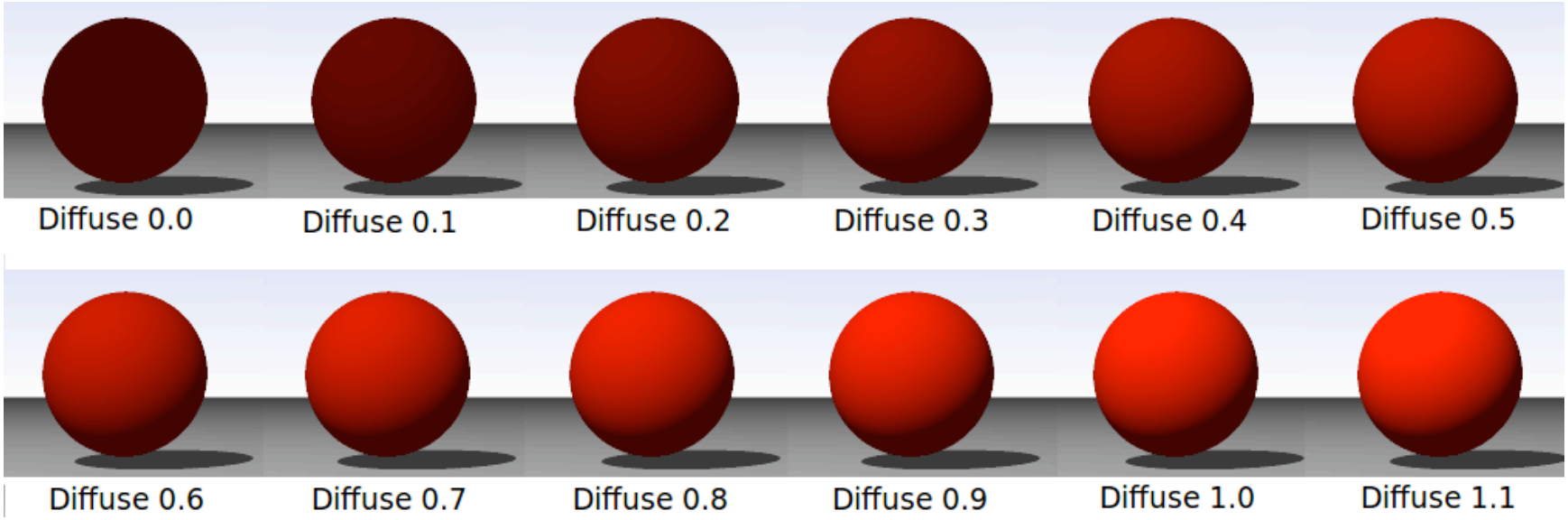
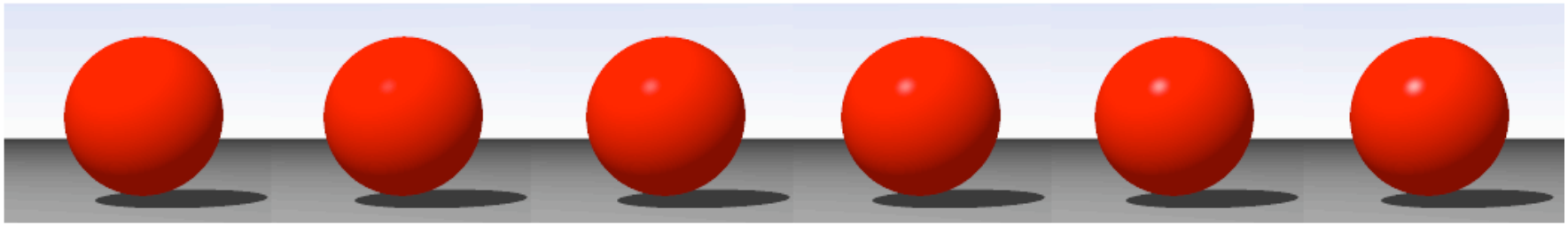
Diffuse property

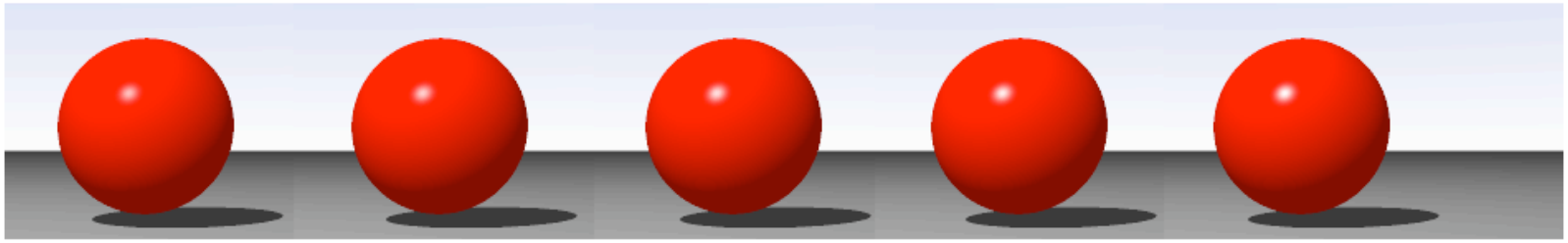
```
sphere {     <0, 1, 2> 1
  pigment{ color Red }
  finish { ambient 0.1 diffuse 0.9 phong 0.8 }
}
```



Phong property

```
sphere {     <0, 1, 2> 1
  pigment{ color Red }
  finish { ambient 0.3 diffuse 0.9 phong 0.8 }
}
```





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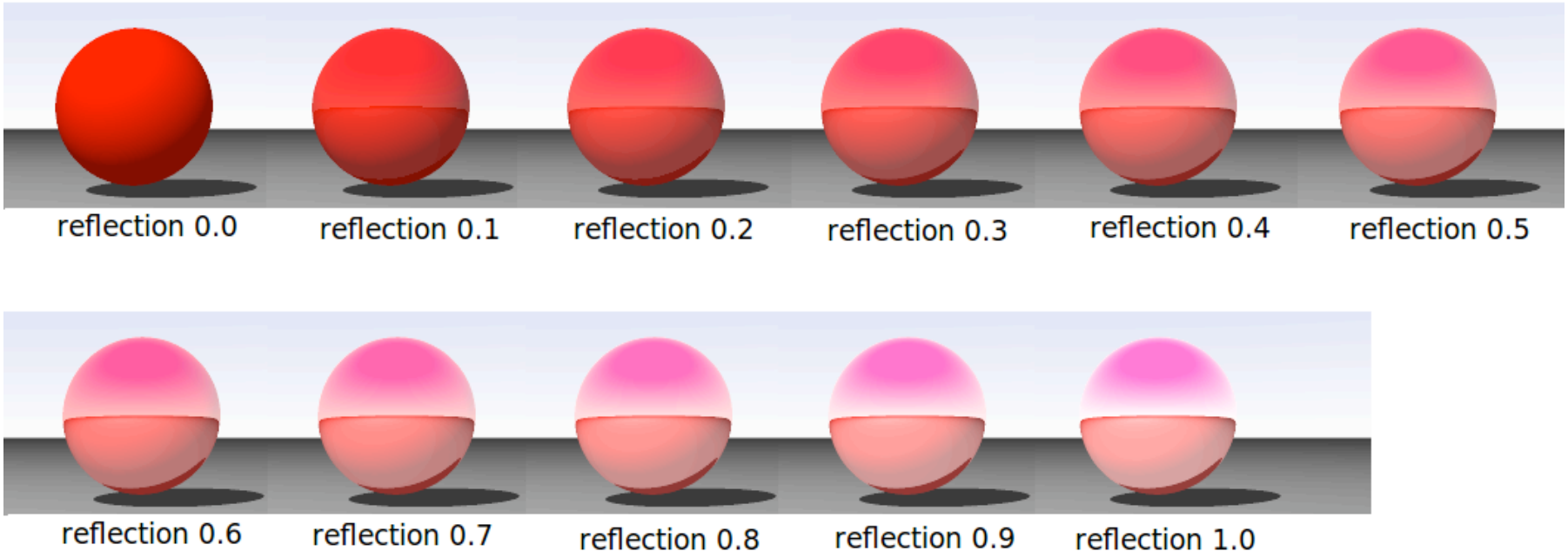
Reflection property



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Default command

It’s laborious to set finish commands every objects every time.

For that case, use default command!!

Usually, following default values are recommended.

```
#default{ finish{ ambient 0.1 diffuse 0.9 phong 1.0}}
```

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How to model molecules?

Molecule is modeled from group of spheres and cylinders.
I made a code to make set of them from xyz format.

1. Source code -> Nanowiki -> pov-mol.c

2. [you@your_PC] gcc pov-mol.c -o povmol -lm

3. [you@your_PC] ./povmol molecule.xyz > mol.inc

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How to model molecules?

4. Edit mol.inc (change color, size of bonds etc)

```
#declare radius_H = 0.400;
#declare radius_C = 0.400;
#declare color_C = rgb<0,0,1>;
#declare color_H = rgb<1,1,1>;

#declare color_bond = rgb<.5,.5,.5>;
#declare radius_bond = 0.200;

#declare molecule1 = union {
   sphere{<     2.09786360,     0.00000000,    -1.24689990> radius_C
texture { pigment{ color_C } finish {phong 1  ambient 0.2 diffuse 0.8} } }
   sphere{<     1.40278720,     0.00000000,    -2.49420100> radius_C
texture { pigment{ color_C } finish {phong 1  ambient 0.2 diffuse 0.8} } }
…
```

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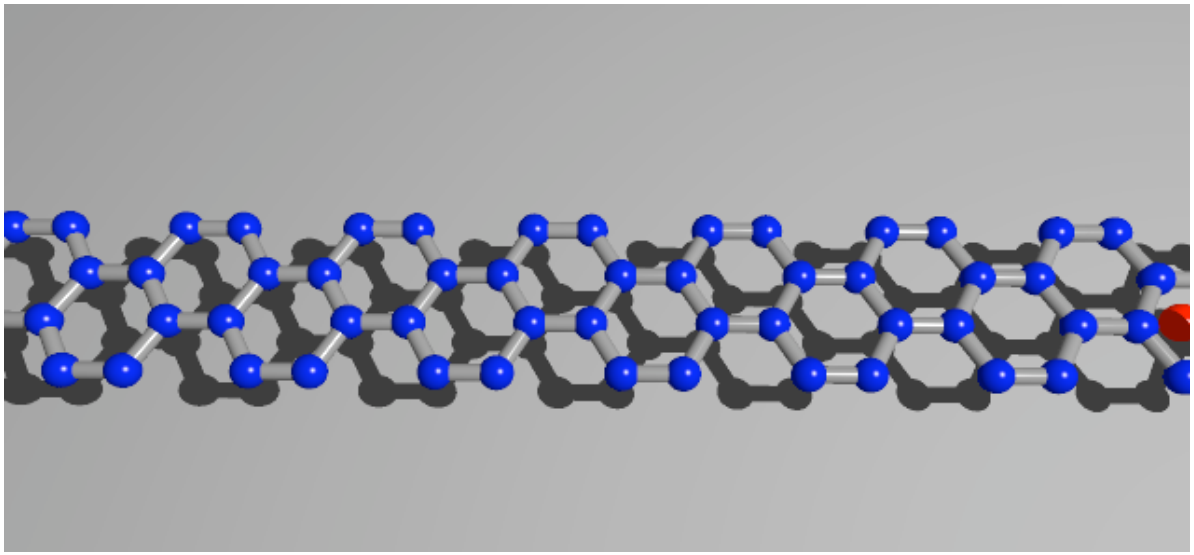
How to model molecules?

5. Include the mol.inc in your pov file
   #include “mol.inc”

6. Call the molecule and its bonds:

```
object{molecule1}
object{molecule1_bond}
```



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Other important options

```
1. translate <1.0, 2.0, 3.0>
2. rotate <0, 90, 0>
3. scale <1,2,1>
4. no_shadow
5. for loop
6. unite
7. #declare
8.
```

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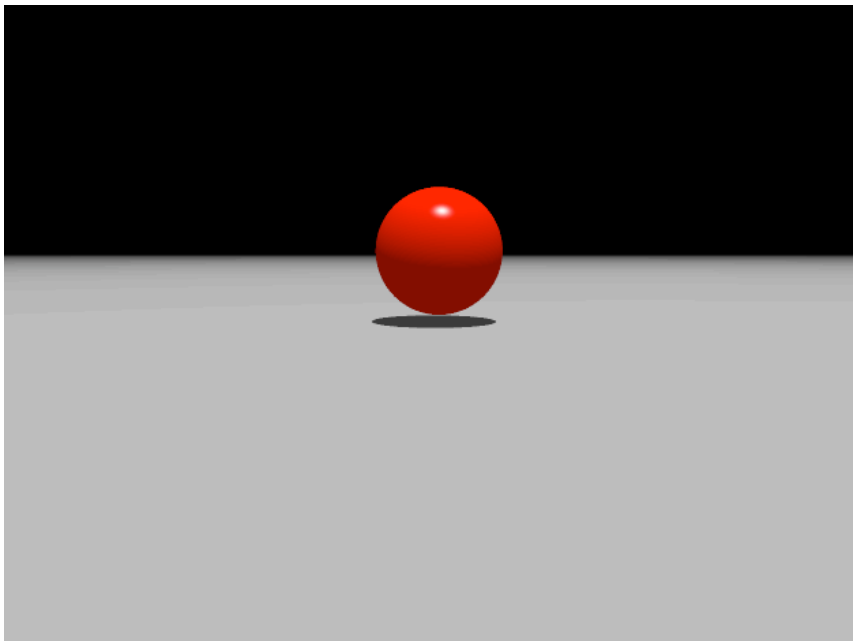
How to set Sky ?

If sky is not defined, your system will look like the scene in the space.



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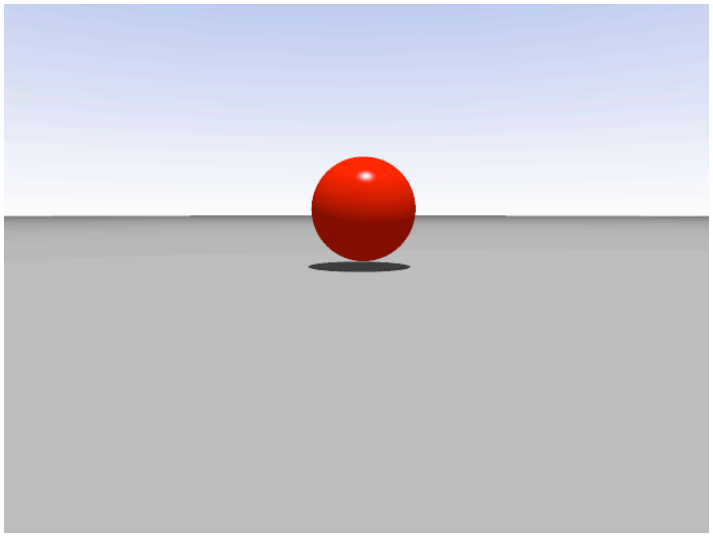
How to set Sky ?

1. Put a large sphere

```
sphere{<0,0,0>,1 hollow
   texture{
      pigment{gradient <0,1,0>
         color_map{
            [0.0 color rgb<1,1,1>]
            [0.8 color rgb<0.1,0.25,0.75>]
            [1.0 color rgb<0.1,0.25,0.75>]
         }
      } // end pigment
      finish {ambient 1 diffuse 0}
   }
   // end of texture
   scale 1000
}
```



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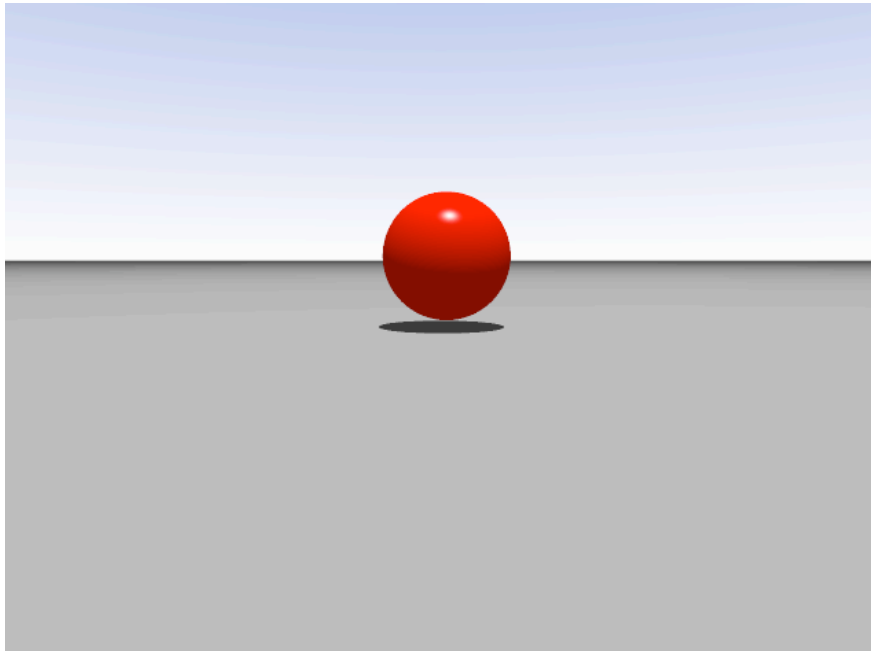
How to set Sky ?

2. Use sky_sphere command

```
sky_sphere{
   pigment{ gradient <0,1,0>
      color_map{
         [0.0 color rgb<1,1,1>]
         [0.8 color rgb<0.1,0.25,0.75>]
         [1.0 color rgb<0.1,0.25,0.75>]
      }
   } // end pigment
} // end of sky_sphere --
```



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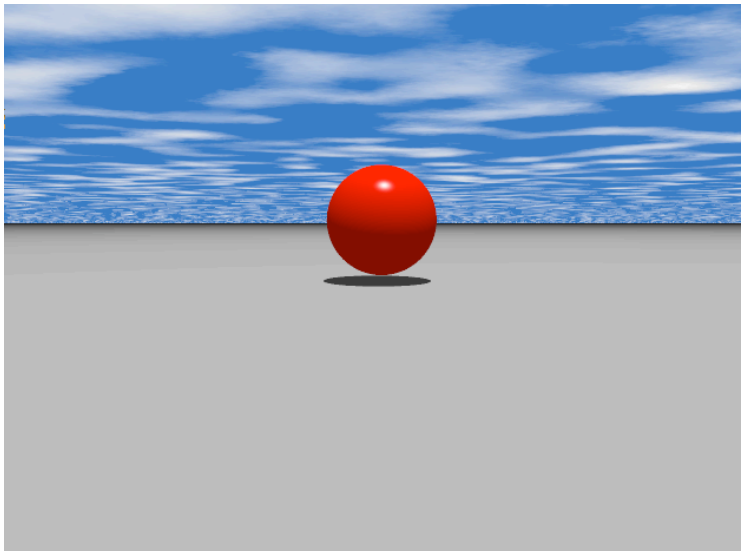
How to set Sky ?

3. Use plane



```
plane{<0,1,0>,1 hollow  //
     texture{
          pigment {color rgb<0.1,0.35,0.8>*0.8}
          finish {ambient 1  diffuse 0}
     } // end texture 1

     texture{
          pigment{ bozo turbulence 0.17
               octaves 6  omega 0.7 lambda 2
               color_map {
                    [0.0  color rgb <0.95, 0.95, 0.95> ]
                    [0.05  color rgb <1, 1, 1>*1.25 ]
                    [0.15 color rgb <0.85, 0.85, 0.85> ]
                    [0.55 color rgbt <1, 1, 1, 1>*1 ]
                    [1.0 color rgbt <1, 1, 1, 1>*1 ]
               } // end color_map
               translate< 3, 0,-1>
               scale <0.3, 0.4, 0.2>*3
          } // end pigment
          finish {ambient 1 diffuse 0}
     } // end texture 2
     scale 10000
}
```

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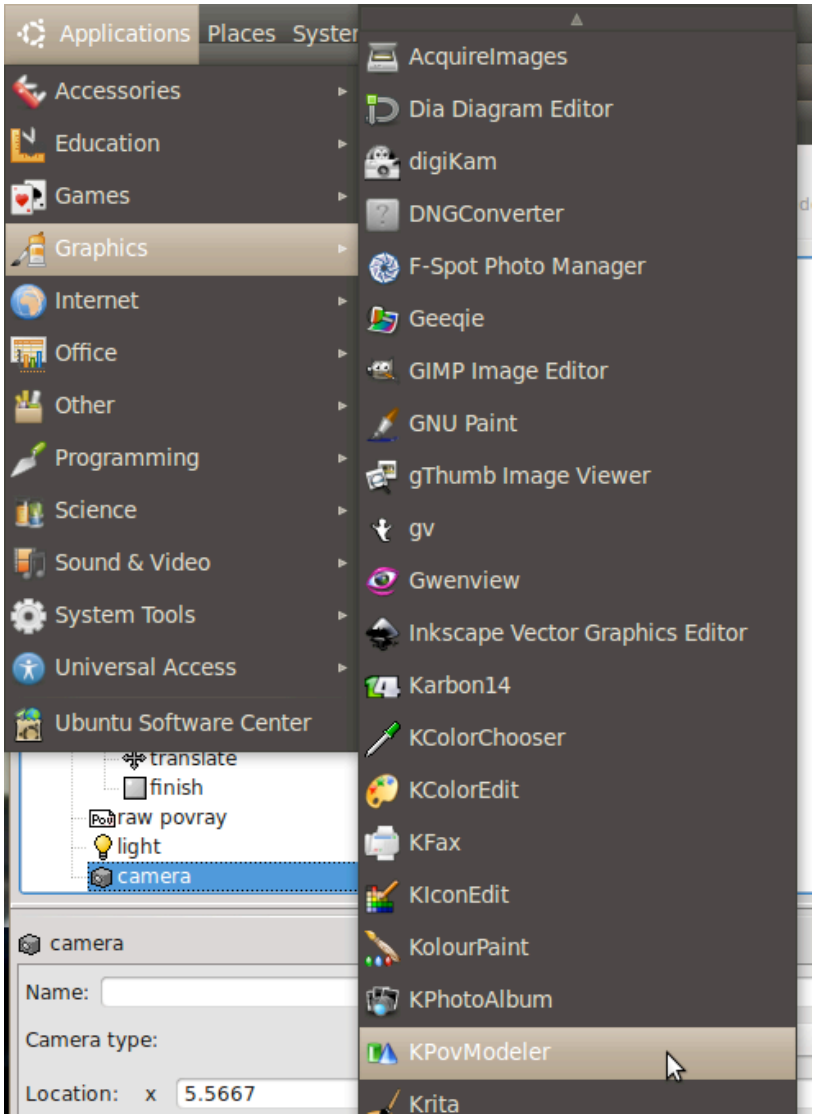
KpovModeller



Ubuntu linux has a nice interactive Povray modeller (GUI).

At HAL, you can use it.

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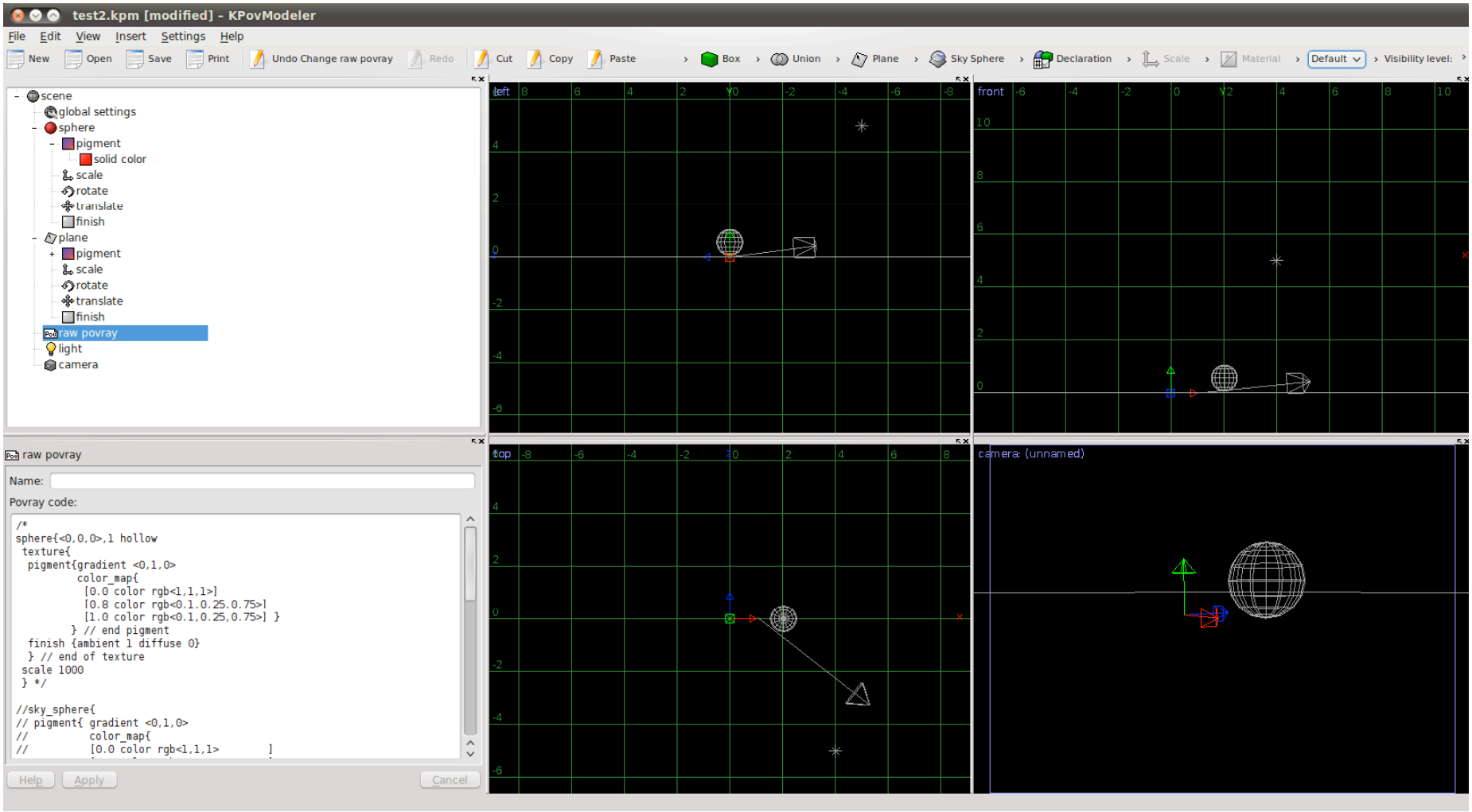
KpovModeller



Thanks!