
Subject: Re: Need an "atom" object

Posted by [Michael Werger](#) on Thu, 01 Apr 1999 08:00:00 GMT

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David Fanning wrote:

>
> Hi Folks,
>
> I'm trying to save myself a bit of time and help out a friend
> at the same time. We are looking for some kind of "atom"
> object that would be a sphere with a particular color
> and radius. It might have its own light source associated
> with it. The idea would be to clump these atoms together
> into a rotatable "molecule", if you like.
>

Hy object'lers,

I re-arranged code from the recent IDL distribution and
put it in some way together what we would think of a simple
atom/molecule demo..

```
IDL> .run cristal
```

```
IDL> cristal
```

be warned: have the examples directories of IDL also in
your searchable path because it uses surf_track.pro (wonderful app)
and orb__define.pro

(Oh' it doesn't work? feedback is appreciated and I will then
return code which should work...)

--

Michael Werger

-----o

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File Attachments

1) [cristal.pro](#), downloaded 133 times

Subject: Re: Need an "atom" object

Posted by [steinhh](#) on Thu, 01 Apr 1999 08:00:00 GMT

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David Fanning wrote:

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> with it. The idea would be to clump these atoms together
> into a rotatable "molecule", if you like.

I think Richard Adams' suggestion of using the "orb" data type would probably fill your needs, David, but just in case you'd like a small, quick'n dirty thing to build on, I made the following implementation of a "ball" object the other day.

Like the "orb" object, it's subclassed from the IDLgrModel class, and contains a polygon object. The surface is built up by a square array, equally spaced in [theta,phi] "space". Input radius r and number of points n.

The polygon vertex list forms a "quad strip" to take advantage of polygon mesh optimization.

I see the "orb" class has an inherent "position", personally I like to implement this through a translation of the "ball" model itself.

Regars,

Stein Vidar

```
-----  
PRO ball::cleanup  
  self->idlgrmodel::cleanup  
END
```

```
FUNCTION ball::init,r,n,color=color  
  
  if n_elements(color) eq 0 then color=[255,255,255]  
  
  dummy = self->idlgrmodel::init()  
  
  x = rebin(reform(findgen(n)/n,n,1,/overwrite),n,n,/sample)  
  y = rebin(reform(findgen(n)/(n-1),1,n,/overwrite),n,n,/sample)
```

```

theta = x*(360.0*!dtor)
phi = (y-0.5)*(180.0*!dtor)

sinphi = sin(phi)
cosphi = cos(temporary(phi))

costheta = cos(theta)
sintheta = sin(temporary(theta))

xp = r* temporary(costheta)*cosphi
yp = r* temporary(sintheta)*temporary(cosphi)
zp = r* temporary(sinphi)

gons = lindgen(5,n*(n-1))

FOR yi=0,n-2 DO BEGIN
  yyi = [yi,yi,yi+1,yi+1]
  FOR xi=0,n-1 DO BEGIN
    xxi = [xi,(xi+1) MOD n,(xi+1) MOD n,xi]
    gons(0,yi*n+xi) = [4,xxi + yyi*n]
  END
END
stop

xp = reform(xp,n*n,/overwrite)
yp = reform(yp,n*n,/overwrite)
zp = reform(zp,n*n,/overwrite)

ball = obj_new('idlgrpolygon',xp,yp,zp,polygons=gons,color=color)

self->add,ball
self->translate,100,0,2*r
return,1
END

PRO ball__define
  dummy = {BALL,$
           INHERITS idlgrmodel $
           }
END

```

Subject: Re: Need an "atom" object
Posted by [Richard J Adams](#) on Thu, 01 Apr 1999 08:00:00 GMT
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Dear David,

Subject: Re: Need an "atom" object
Posted by [rmlongfield](#) on Fri, 02 Apr 1999 08:00:00 GMT
[View Forum Message](#) <> [Reply to Message](#)

In article <37036F0B.2ABBE82F@astro.estec.esa.nl>,
Michael Werger <mwerger@astro.estec.esa.nl> wrote:

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> return code which should work...)

Hi Michael,

Just tried your program and it works on a Silicon Graphics with IDL5.2
(Once I realized that the name was cristal and not crystal :-).
The code looks very simple and its almost tempting to start learning objects.
I found just one problem when I pressed the right button:

```
% Tag name WLABEL is undefined for structure <Anonymous>.  
% Execution halted at: CRISTAL_EVENT    91  
/usr/people/dlhopols/IDL/crystal.pro  
%           WIDGET_PROCESS_EVENTS  
%           $MAIN$
```

Also, after the error, I couldn't delete the widget at all and had to exit
IDL. Is there a command that would do this from within IDL?

Rose

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