

Subject: Re: AtomEye**From:** Branden Kappes <bkappes@mines.edu>**Date:** Mon, 21 Apr 2008 11:47:43 -0600**To:** Ju Li <liju@seas.upenn.edu>

Ju,

Thanks for putting up with my questions. I was able to eliminate the problem and have included the patch file for the AX directory. This should be run from the Src-20060530 directory.

```
patch -p0 < AX.patch
```

I apologize if this is not the most effective way of doing this. I am new to patching as well (all my development to this point has been just that--my development).

Thanks again for your help with this and especially for AtomEye.

-Branden

Ju Li wrote:

Thanks for the investigation, Branden. At your level, you should be able to find and correct the problem soon.

Do you think

```
/* recombining floats */
#define AX_pixel(r,g,b) ( \
    0xff000000 | \
    (AX_PIXEL(r)&AX_rmask) | \
    (AX_PIXEL(g)&AX_gmask) | \
    (AX_PIXEL(b)&AX_bmask) )
```

might help?

Dear Ju,

Thank you for your reply.

I tried disabling transparency, but that did not resolve the problem. I think the error messages result because the masks reported by the X11 Visual struct on my system:

```
red_mask = 0xff ff 00 00, green_mask = 0xff 00 ff 00, blue_mask = 0xff 00 00 ff (spaces
added for readability)
```

do not match the values from "rgb.txt" since the values from the color table do not include the alpha mask (I verified this). As a result, when the named colors are read from rgb.txt, we get

```
red = 0xff 00 00, green = 0xff 00, and blue = 0xff
```

The comparison made in Scan.c checks (in my nomenclature)

```
if(red_mask != red) { /* prints error message */ }
etc.
```

I tried dropping the alpha mask from "AX_rmask", "AX_gmask", and "AX_bmask", e.g. changing AX_rmask from 0xFF FF 00 00 (as reported by Visual*) to 0xFF 00 00 (as would be read from rgb.txt)

This got rid of the error messages, but did not fix the transparency issue. Similarly, I tried adding the alpha mask to "AX_pixel(r, g, b)" which, again, eliminated the message but did not fix the transparency problem.

While trying to nail down the problem, I ran across

```
#define AX_COLORPIXEL(c) \
    AX_ColorPixel(iw, (c)>>16, ((c)>>8)&0xFF, (c)&0xFF, 0xFF)
```

which seems to assume that $c \leq 0xFF\ FF\ FF$ which, as we see with red_mask, green_mask, and blue_mask, is not necessarily the case. I tried changing this (and analogously, AX_COLORCARRIER) to

```
#define AX_COLORPIXEL(c) \
    AX_ColorPixel(iw, ((c)>>16)&0xFF, ((c)>>8)&0xFF, (c)&0xFF, 0xFF)
```

but, again, to no avail. Nothing I tried changed the output--that is, I did not see a change

in hue or opacity from any of these changes. One thing that stands out from the error message: colormap id = 0x3 E0 00 01 > 0x FF FF FF and would account for the low opacity (~1.25%).

Thank you,

-Branden

Ju Li wrote:

Dear Branden,

I have never dealt with semi-transparent window before. So this might be the reason for the complaint message. If you change the window manager or disallow transparency, does the problem go away?

Ju.

Dr. Li,

I am a Ph.D. student at the Colorado School of Mines and, up until recently, I have been using RasMol to visualize my MD/MC simulation results when my advisor (Dr. Moneesh Upmanyu) suggested AtomEye.

I have used it without trouble on my PowerBook G4, but when I use the i686 binary or compile from source on my Linux box (running Ubuntu 7 "Gutsy Gibbon" on an AMD 64-bit Opteron) I get the following errors:

```
<quote>
colormap id = 0x3e00001
ff0000 ffff0000
AX_plugin_Scan_module: red mask not working

colormap id = 0x3e00001
ff00 ff00ff00
AX_plugin_Scan_module: green mask not working

colormap id = 0x3e00001
ff ff0000ff
AX_plugin_Scan_module: blue mask not working
</quote>
```

At this point AtomEye continues to run, but only white is fully opaque (presumably). In front of a semi-transparent xterm window, the colors of the atoms are visible, but partially transparent. In front of an opaque window, the atoms are completely transparent. I tried to hack the AtomEye code, but I have no experience with programming for X11. I was able to eliminate the error messages quoted above by adding an alpha mask to AX_pixel in AX.h, but I could not resolve the transparency issue. I have taken a couple screenshots that demonstrate this and have included them in this email.

Any help you can provide would be greatly appreciated.

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```
diff -Naur AX/AX.c AX_new/AX.c
--- AX/AX.c      2006-01-11 16:53:34.000000000 -0700
+++ AX_new/AX.c  2008-04-21 10:51:44.000000000 -0600
@@ -429,9 +429,9 @@
     ( AX_visual[iw]->class == TrueColor );
     if ( AX_noneedcolormap )
     {
-        AX_rmask = AX_visual[iw] -> red_mask;
-        AX_gmask = AX_visual[iw] -> green_mask;
```

```

-         AX_bmask = AX_visual[iw] -> blue_mask;
+         AX_rmask = AX_visual[iw] -> red_mask & AX_COLORMASK;
+         AX_gmask = AX_visual[iw] -> green_mask & AX_COLORMASK;
+         AX_bmask = AX_visual[iw] -> blue_mask & AX_COLORMASK;
    }

#ifdef _AX_USE_SHM
diff -Naur AX/AX.h AX_new/AX.h
--- AX/AX.h      2006-01-11 16:53:34.000000000 -0700
+++ AX_new/AX.h  2008-04-21 11:16:12.000000000 -0600
@@ -68,6 +68,8 @@
    #define AX_DEFHEIGHT  AX_DEFWIDTH

    /* named colors: provided by AX gratis */
+   #define AX_ALPHAMASK  0xFF000000
+   #define AX_COLORMASK  0x00FFFFFF
    #define AX_NAMEDCOLORS 8
    #define AX_BLACK      0
    #define AX_RED        1
@@ -372,7 +374,8 @@
    extern AX_Pixel AX_namedpixel [AX_NAMEDCOLORS];

    /* recombining floats */
-   #define AX_pixel(r,g,b) ( \
+   #define AX_pixel(r,g,b) ( \
+   (AX_ALPHAMASK) | \
        (AX_PIXEL(r)&AX_rmask) | \
        (AX_PIXEL(g)&AX_gmask) | \
        (AX_PIXEL(b)&AX_bmask) )
@@ -386,7 +389,7 @@

    /* 0xFFFFFFFF interface */
    #define AX_COLORPIXEL(c) \
-   AX_ColorPixel(iw, (c)>>16, ((c)>>8)&0xFF, (c)&0xFF, 0xFF)
+   AX_ColorPixel(iw, ((c)>>16)&0xFF, ((c)>>8)&0xFF, (c)&0xFF, 0xFF)

    /** AX_Carrier: interface to Direct Pixmap Access like AX_set() **/
    extern AX_Carrier AX_namedcarrier [AX_NAMEDCOLORS];
@@ -424,7 +427,8 @@

    /* recombining floats */
-   #define AX_carrier(r,g,b) ( \
+   #define AX_carrier(r,g,b) ( \
+   (AX_ALPHAMASK) | \
        (AX_CARRIER(r)&AX_rmask) | \
        (AX_CARRIER(g)&AX_gmask) | \
        (AX_CARRIER(b)&AX_bmask) )
@@ -439,7 +443,7 @@

    /* 0xFFFFFFFF interface */
    #define AX_COLORCARRIER(iw,c) \
-   AX_ColorCarrier(iw, (c)>>16, ((c)>>8)&0xFF, (c)&0xFF, 0xFF)
+   AX_ColorCarrier(iw, ((c)>>16)&0xFF, ((c)>>8)&0xFF, (c)&0xFF, 0xFF)

    /* Mixing two color carriers */
    #define AX_mix(c0,c1,a1) AX_carrier( \
@@ -1704,7 +1708,10 @@
        AX_Float      z;
    } AX_3D_Pixel;

-   #define AX_3D_AssignRGB(P,R,G,B) ((P).r=(R),(P).g=(G),(P).b=(B))
+   #define AX_3D_AssignRGB(P,R,G,B) ( \
+   (P).r=(R), \
+   (P).g=(G), \
+   (P).b=(B))

    /*****/
    /* Line Support */

```

AX.patch

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