

Subject: AtomEye
From: Branden Kappes <bkappes@mines.edu>
Date: Thu, 17 Apr 2008 17:20:53 -0600
To: liju@seas.upenn.edu

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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The screenshot shows a Linux desktop with a terminal window, a file manager, and a molecular visualization window. The terminal window displays the output of the AtomEye program, showing various warnings and error messages related to colormap and plugin issues. The file manager shows a directory listing of files and folders. The molecular visualization window displays a 3D model of a molecule, with a coordinate system and various statistics.

Terminal Window Output:

```
LeastSquareStrain.c:10: warning: (near initialization for 'ref[0]')
g77 -D linux -Wall -O3 -m64 -march=x86-64 -mmmx -msse -ffast-math -funroll-loops -fomit-frame-pointer -I/home/bkappes/Co/Include -A.o primitives.o viewport.o utils.o xtal_shift.o info.o rot_patch.o scratch.o geo.o LeastSquareStrain.o -o A -L/home/bkappes/Co/Lib -LAX -lpng -lz -ljpeg -latoms -lVecMat3 -lVecMat -lIO -lScalar -lTimer -llapack -lblas -lXpm -lreadline -lhistory -ltermcap -lm -ldl -lX11 -lXt -lXmu -lX11R6/lib/ -lXext -lX11 -lpthread
/home/bkappes/Co/Lib/LibAX.a(AX.o): In function 'AX_save_pixmap_as_eps':
AX.c:(.text+0x1794): warning: the use of 'tmpnam' is dangerous; better use 'mkstemp'
Current time on solomon: Apr 17 17:18
-rwxr-xr-x 1 bkappes bkappes 971296 2008-04-17 17:18 /Co/Bin/A
===== Running "A 1D66.pdb.bz2" ===== Really heavy users may try out
colormap id = 0x3c00001
ff0000 ffff0000
AX_plugin_Scan_module: red mask not working
colormap id = 0x3c00001
ff00 ff00ff00
AX_plugin_Scan_module: green mask not working
colormap id = 0x3c00001
ff ff0000ff
AX_plugin_Scan_module: blue mask not working
```

File Manager: Shows a directory listing of files and folders, including '2006-july.txt.gz', '20060530-A3.20060602.patch', 'Src-20060530.tar.gz', and 'cnt8x3.cfg'.

Molecular Visualization Window: Displays a 3D model of a molecule, with a coordinate system and various statistics. The window title is '1D66'.

Features:

- order N in both execution time and memory used, where N is the number of atoms
- condensed-matter systems, no problem with >1 million atoms
- auto-detect 8, 16 and 32-bit shared memory or remote memory
- multiple resizable windows in POSIX threads; 0% CPU overhead
- geometrically exact area-weighted antialiasing for atoms
- fast rendering of atoms by caching pixel- and z-maps
- quick toggle between parallel and perspective projection
- full 3-D navigation
- support periodic boundary conditions
- support PDB input file format
- support arbitrary-precision and extendable CFG input
- dynamics simulations
- auto-decompress gzip- or bzip2-compressed input configuration files
- JPEG, PNG and high-resolution EPS screenshots
- customizable atom radii and coloring schemes
- coordination number color-encoding with customizable cutoff radii and invisibility controls
- local atomic von Mises shear strain invariant color-encoding
- user-defined property color-encoding, in hsv, jet, and other colormapping choices
- color-marking an initial configuration to track subsequent atomic displacements
- cooperative X-terminal input with GNU readline / history
- up to 16 arbitrary cutting planes with advancing / rotation / flipping controls
- animation script for making movies

The screenshot displays the AtomEye application interface. The main window is titled "bkappes@solomon: ~/Software/AtomEye/Src-20060530/A". It contains a terminal window on the left with the following output:

```
LeastSquareStrain.c:10: warning: (near initialization for 'ref[0]')
g77 -D_Linux -Wall -O3 -m64 -march=x86-64 -mmmx -msse -ffast-math -funroll-loops
-fomit-frame-pointer -I/home/bkappes/Co/Include -A.o primitives.o viewport.o
utils.o xtal_shift.o info.o rcut_patch.o scratch.o geo.o LeastSquareStrain.o
-o A -L/home/bkappes/Co/Lib -lAX -lpng -lz -ljpeg -lAtoms -lVecMat3 -lVecMat -l
IO -lScalar -lTimer -llapack -lblas -lxpm -lreadline -lhistory -ltermcap -lm -F
/usr/X11R6/lib/ -lXext -lX11 -lpthread
/home/bkappes/Co/Lib/LibAX.a(AX.o): In function
AX.c:(.text+0x1794): warning: the use of 'tmpn
emp'
Current time on solomon: Apr 17 17:
-rwxr-xr-x 1 bkappes bkappes 971296 2008-04-17
Teplot 8.0 CMSN 200
===== Running "A 1D66.pdb.bz2" =====
colormap id = 0x3c00001
ff0000 ffff0000
AX_plugin_Scan_module: red mask not working
colormap id = 0x3c00001
ff00 ffff00
AX_plugin_Scan_module: green mask not working
colormap id = 0x3c00001
ff ffff00
AX_plugin_Scan_module: blue mask not working
```

The central window shows a 3D molecular model of a protein structure, labeled "1D66". The right window displays statistics for the 1D66 structure:

```
max=4, min=0, avg=1.04 (7.1%), std.dev.=0.63 (4.3%),
Compressed atom-atom list: 1762 entries, 14372 bytes allocated,
max=4, min=0, avg=1.04, std.dev.=0.63 (60.2%),
All bin-related allocations freed,
----- Coordination Number Statistics -----
Coord. Count Percentage R G B Name
0 51 2.83% 1.000 1.000 1.000 white
1 416 23.61% 0.251 0.878 0.816 turquoise
2 686 38.88% 0.871 0.722 0.529 burlywood
3 570 32.35% 0.133 0.545 0.133 ForestGreen
4 36 2.04% 0.745 0.745 0.745 gray
5 4 0.23% 1.000 0.000 0.000 red
-----
average = 2.07719, most populous = 2,
avg. M = | 1.056038 -0.009179 0.008883 |
| -0.009179 0.754673 -0.028411 |
| 0.008883 -0.028411 1.020723 |
avg. microscopic shear strain = 0.0838333
This process has used up to 2.74 MB.
```

The bottom window shows a list of downloaded files:

- 2006-july.txt.gz Done
- 20060530-A3.20060602.patch Done
- Src-20060530.tar.gz Done
- cnt8x3.cfg

The status bar at the bottom shows the application is running on "AtomEye: atomistic ...".

omEye, so your colleagues may know about this free tool. Thank

Screenshot1.png

Content-Type: image/png
Content-Encoding: base64

Screenshot2.png

Content-Type: image/png
Content-Encoding: base64