

**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 the following elements:

- Terminal Window:** Displays the output of running AtomEye. It shows several error messages: "AX\_plugin\_Scan\_module: red mask not working", "AX\_plugin\_Scan\_module: green mask not working", and "AX\_plugin\_Scan\_module: blue mask not working". A warning message states: "warning: the use of 'tmpnam' is dangerous; better use 'mkstemp'".
- 1D66 Window:** Shows a table of coordination number statistics. The table has columns for Coord., Count, Percentage, R, G, B, and Name. The data is as follows:
 

Coord.	Count	Percentage	R	G	B	Name
0	51	2.83%	1.000	1.000	1.000	white
1	415	23.61%	0.251	0.878	0.816	turquoise
2	686	38.83%	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

 Summary statistics: average = 2.07719, most populous = 2.
- File Manager:** Shows a list of downloaded files: 2006-July.txt.gz, 20060530-A3.20060602.patch, Src-20060530.tar.gz, and cnt8x3.cfg.
- Search Bar:** Located at the bottom of the desktop, with a search box and options for "Next", "Previous", "Highlight all", and "Match case".

The screenshot displays the AtomEye application window with a 3D visualization of a molecular structure. A terminal window in the background shows the execution of the program with various command-line options and output for a file named '1D66'. The terminal output includes statistics on atom coordination and memory usage.

```

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.

```

Below the terminal window, a list of features is provided:

- order  $N$  in both execution time and memory used, where  $N$  is the number of atoms; designed for condensed-matter systems, no problem with  $>1$  million atoms
- auto-detect 8, 16 and 32-bit shared memory or remote X-displays
- multiple resizable windows in POSIX threads; 0% CPU usage if not moving
- geometrically exact area-weighted antialiasing for atoms, bonds, and wireframes
- fast rendering of atoms by caching pixel- and z-maps in the main memory
- quick toggle between parallel and perspective projections
- full 3-D navigation
- support periodic boundary conditions
- support PDB input file format
- support arbitrary-precision and extendable CFG input file format for large-scale, reloadable molecular 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

AtomEye, 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