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.

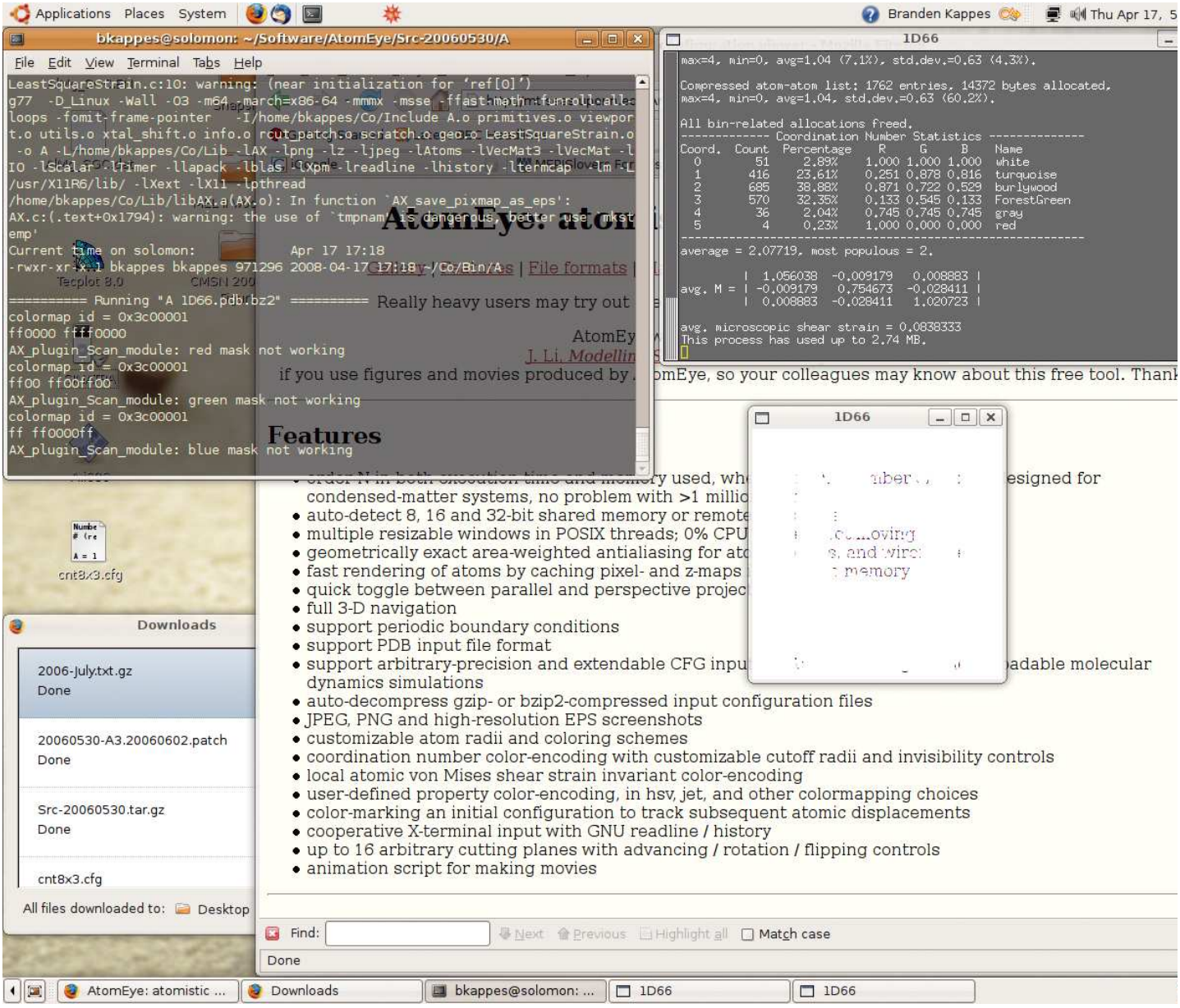
I have used it without trouble on my PowerBook G4, but when I use the i686 binary or compile from source on my Linux box (running Ubuntu 7 "Gutsy Gibbon" on an AMD 64-bit Opteron) I get the following errors:

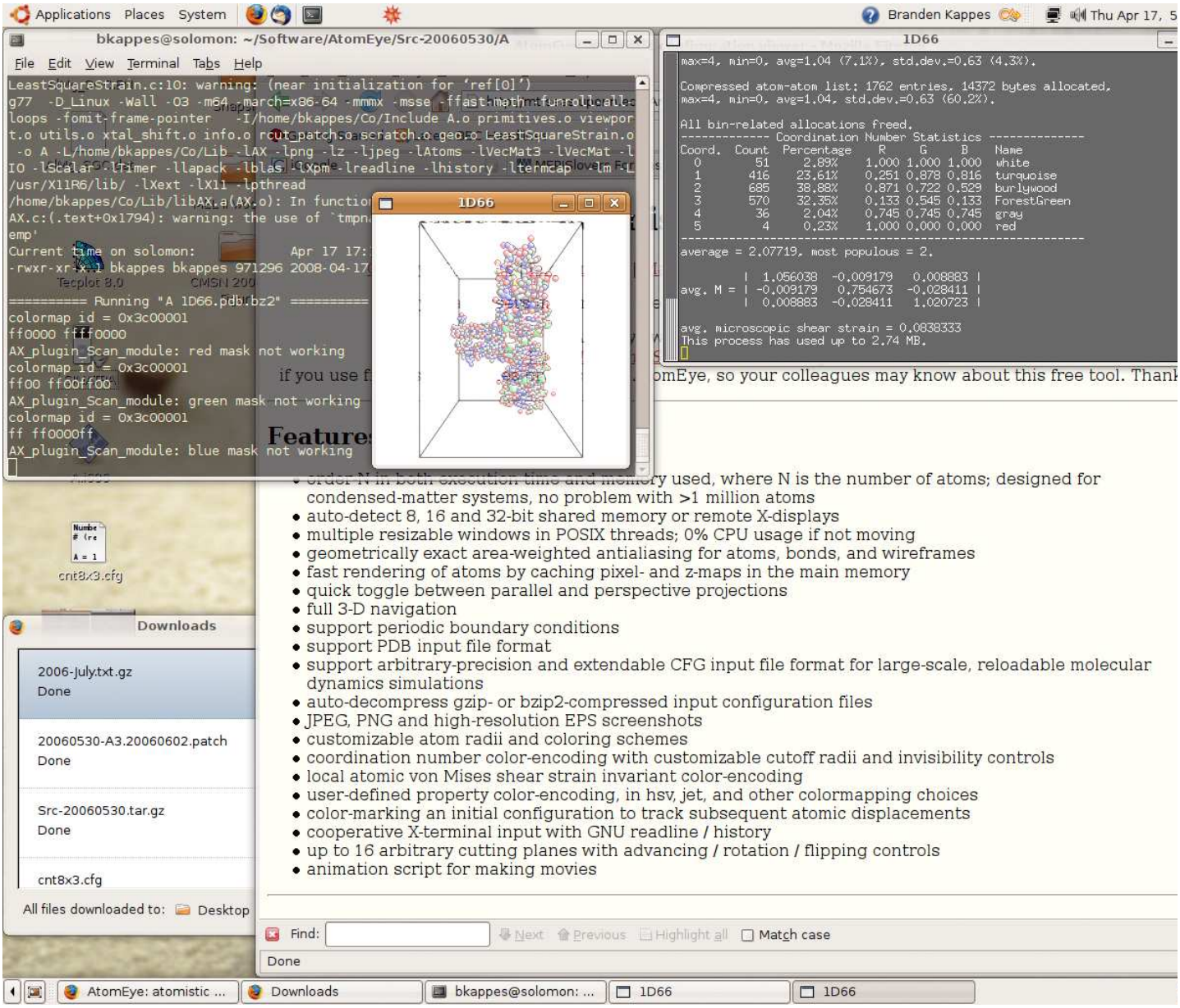
<quote>
```
colormap id = 0x3e00001
ff0000 ffff0000
AX_plugin_Scan_module: red mask not working

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.

Branden Kappes
Ph.D. Candidate
Colorado School of Mines
1600 Illinois St.
Golden, CO 80401
bkappes@mines.edu





- 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

Screenshot1.png	Content-Type: image/png Content-Encoding: base64

Screenshot2.png	Content-Type: image/png Content-Encoding: base64