

Lammps animations with atomeye (generation of movie files)

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tool: lmp2cfg contained in lammps tar file generates cfg files from lammps dump files as inputs for atomeye.
and atomeye generates jpeg files from these inputs.
then avi movie files can be obtained with ffmpeg.

intsllation of atomeye

obtaining binary for os x from [AtomEye: atomistic configuration viewer](#) and copy it to a directory a directory that execute path is attached to.

intsllation of ffmpeg

atomeye generates every frame of animation as jpeg file. ffmpeg can generate avi movie files from jpeg files.

see [FFmpeg on Mac OS X How-to: Installing and using FFmpeg on Mac OS X](#) for the instllation.

Remark: it is sufficient to install LAME and FFMPEG. you need xcode for the installation. see [Mac Dev Center - Apple Developer](#).

intsllation of lmp2cfg

lmp2cfg.f is included in tools directories of the lammps tar file.
example for the input of lmp2cfg.f

```
400          #total number of atoms in system (may be more than in
dump)
1            #number of atom types in your LAMMPS file
'dumpfile'  #name of the LAMMPS dump file, you need the ' '
1           #first frame
100         #last frame
1           #first atom type
12.0107     #atomic weight
'C'         #atom name
```

usage:

```
gfortran -O -o lmp2cfg lmp2cfg.f
./lmp2cfg < input.txt
```

then files with the extension ".cfg" shall be generated.

a bug fixed code of lmp2cfg: [lmp2cfg.f](#)

gfortran for os x is contained in gcc of
<http://hpc.sourceforge.net>. Gcc-4.7 is recommended.

atomeye operation

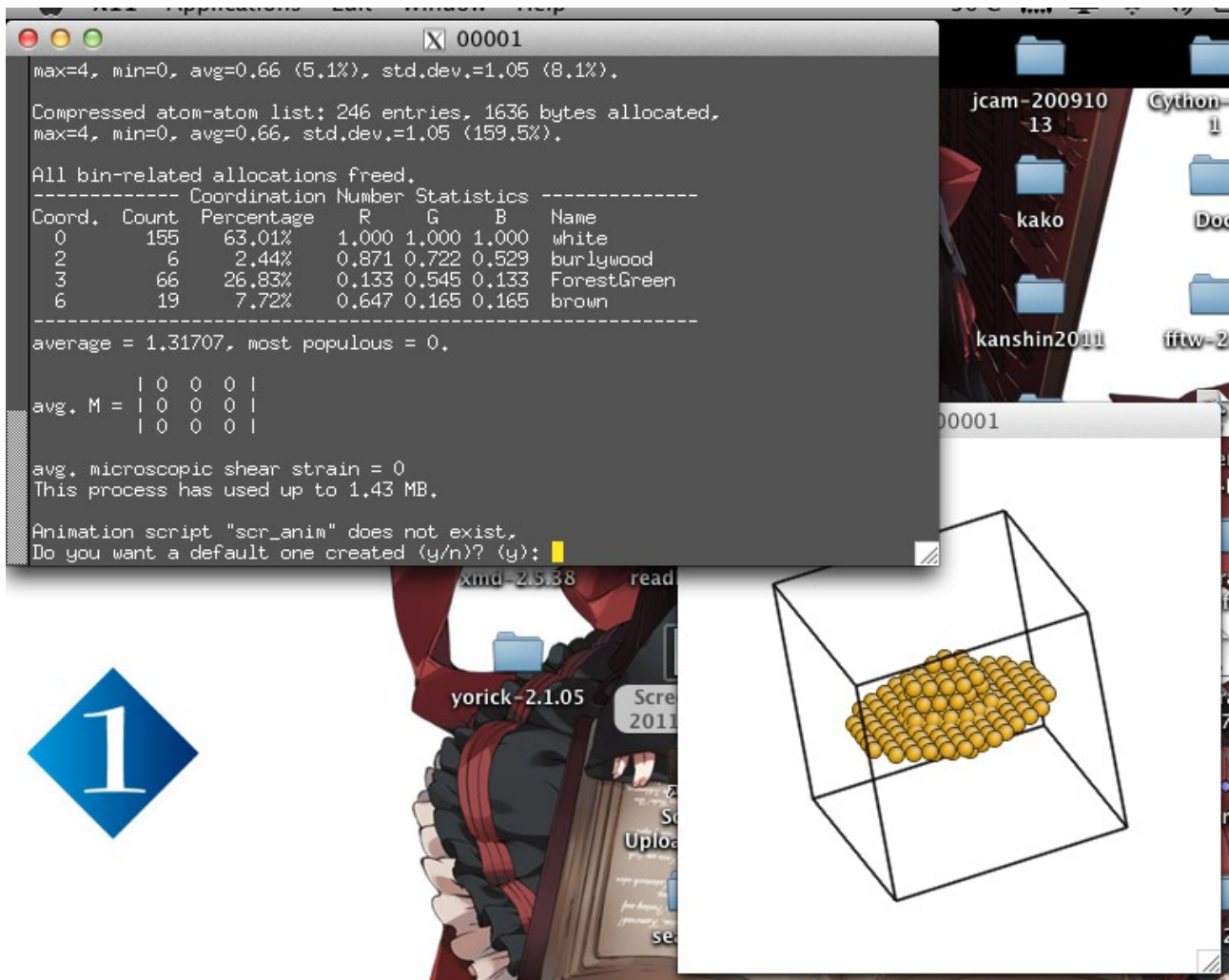
on terminal:

atomeye 00001.cfg &

atomeye on X11:

press "y" on window of a molecular image and press enter-key on the console in X11 of atomeye

then jpeg files (00001.jpg, 00002.jpg, ...) are generaeted in the Jpg folder.



ffmpeg operation --- generating avi files

on terminal: move to the Jpg directory and
`$ ffmpeg -r 12 -i "%05d.jpg" -vcodec mjpeg xenon_bubble.avi`
 (where "-r 12" is a frame rate per second. "-i %05d.jpg" means a sequence of jpeg files started from "00001.jpg")

results for avobe as movies:

[shrinking xenon bubble \(xenon only visible\)](#)

[spreading xenon bubble \(xenon only visible\)](#)

```
Jpg — Terminal — MacBook — bash — 100x30
[3]+ Done
atomeye 00001.cfg (wd: ~/Sites/math/lammps/tools/atomeye/cfg)
(wd now: ~/Sites/math/lammps/tools/atomeye/cfg/Jpg)
MacBook2009:Jpg chibaf$ ffmpeg -r 12 -i "%05d.jpg" -vcodec mjpeg -sameq xenon_bubble.avi
FFmpeg version SVN-r26402, Copyright (c) 2000-2011 the FFmpeg developers
built on Feb 13 2011 07:29:30 with gcc 4.2.1 (Apple Inc. build 5664)
configuration: --enable-libmp3lame --enable-shared --disable-mmx --arch=x86_64
libavutil 50.36.0 / 50.36.0
libavcore 0.16.1 / 0.16.1
libavcodec 52.108.0 / 52.108.0
libavformat 52.93.0 / 52.93.0
libavdevice 52.2.3 / 52.2.3
libavfilter 1.74.0 / 1.74.0
libswscale 0.12.0 / 0.12.0
[image2 @ 0x10100b000] max_analyze_duration reached
Input #0, image2, from '%05d.jpg':
Duration: 00:00:17.50, start: 0.000000, bitrate: N/A
Stream #0.0: Video: mjpeg, yuvj420p, 338x332 [PAR 1:1 DAR 169:166], 12 fps, 12 tbr, 12 t
bc
[buffer @ 0x100c02700] w:338 h:332 pixfmt:yuvj420p
Output #0, avi, to 'xenon_bubble.avi':
Metadata:
ISFT : Lavf52.93.0
Stream #0.0: Video: mjpeg, yuvj420p, 338x332 [PAR 1:1 DAR 169:166], q=2-31, 200 kb/s, 12 tbn, 12
tbc
Stream mapping:
Stream #0.0 -> #0.0
Press [q] to stop encoding
frame= 210 fps= 0 q=1.0 Lsize= 3305kB time=17.50 bitrate=1547.0kbits/s
video:3294kB audio:0kB global headers:0kB muxing overhead 0.322742%
MacBook2009:Jpg chibaf$
```

Figure: Operation of ffmpeg

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