

# computation of lattice parameters of UO2 for temperatures

lattice parameters of  $UO_2$  for temperatures (from 250K to 3000K; step size=125K) were computed.

lammps computed each volume corresponding to each temperature.

lattice parameter was computed as follows:

```
c = (initial volume of system)**(1/3)/5.47 # where 5.47 is an initial lattice parameter.
```

```
lattice parameter at this temperature = (volume at this temperature)**(1/3) / c
```

volume at each temperature was computed with following script:

common header, script\_part1.txt used in the python code below

```
#Initialization:
atom_style charge
units metal
boundary p p p # impose periodic boundary conditions for three directions
dimension 3
newton on
#default is on
#Atom definition:
read data data.fcc111 # uo2 system on fcc 111 lattice
mass 1 238
group 1 type 1
mass 2 16
group 2 type 2
#Force fields:
pair_style hybrid/overlay born/coul/long 10.0 Morse 10.0
pair coeff 1 1 born/coul/long 0.013806784 0.32702 3.26 0.0 0.10 10.0
pair coeff 1 2 born/coul/long 0.013806827 0.327021 3.54 0.0 0.10 10.0
pair coeff 1 2 Morse 1.65 2.369 10.0
pair coeff 2 2 born/coul/long 0.013806869 0.327022 3.82 3.950633264 0.0 0.10 10.0
# the potentials above referred to [lammps-users] Uranium_dioxide,_incorrect_net_charge_of_system
kspace_style ppm 1.0e-4 # use ewald method
```

download: [script\\_part1.txt](#)

the python code, lattice.py: it generates lammps scripts and executes them in a loop

```
#!/usr/bin/python

import sys
from string import *
import os
from subprocess import *

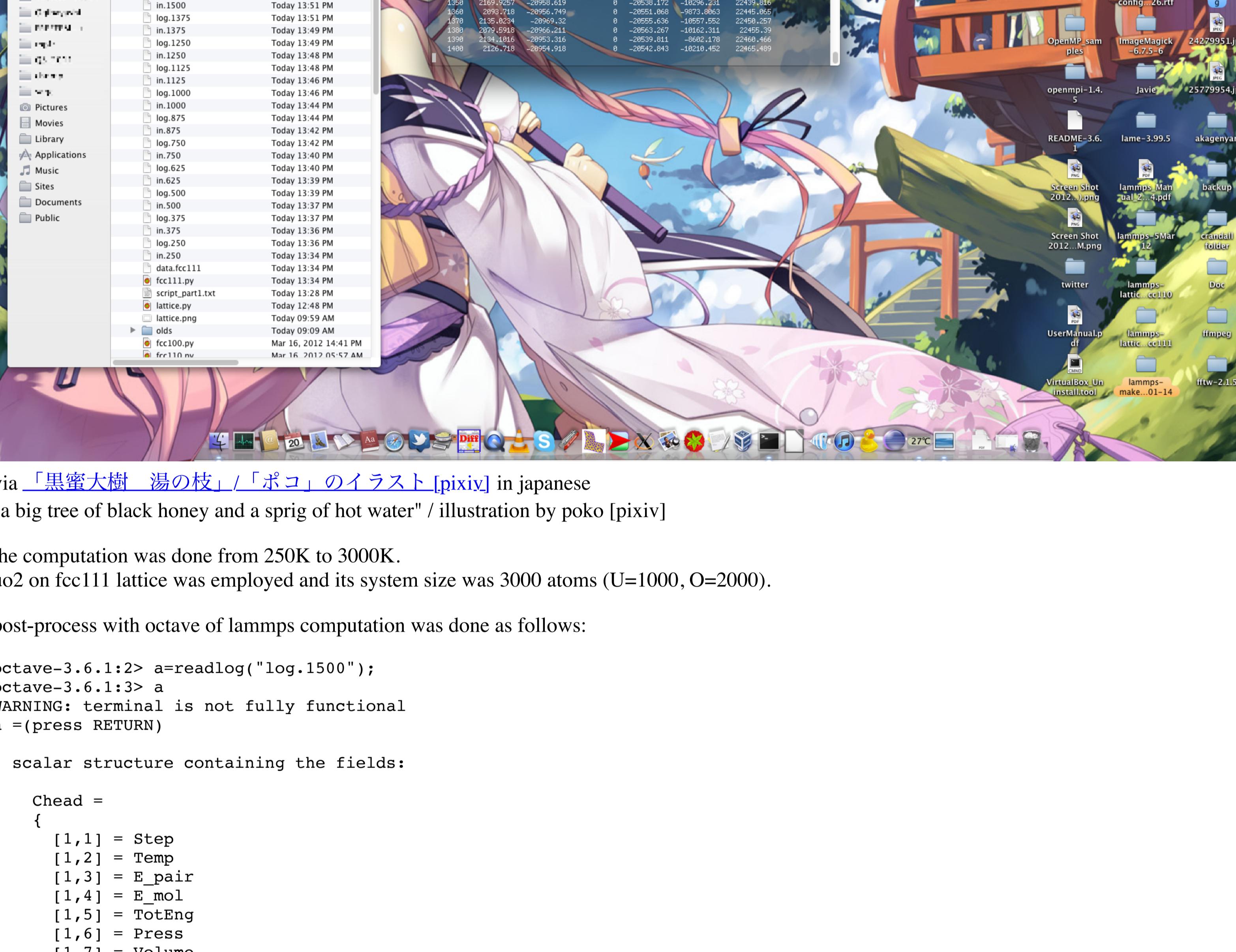
for i in range(0,23):
    temp=250+i*125
    fn="script1"+str(temp)
    call("echo '#' >"+fn, shell=True) # use the header above
    s="#log log "+str(temp)+" "
    call("echo "+s+">"+fn, shell=True)
    s="velocity all create "+str(float(temp))+ " 78621 dist gaussian"
    call("echo "+s+">"+fn, shell=True)
    s="fix NPT all npt temp "+str(float(temp))+ " "+str(float(temp))+ " 0.005 iso 0.0 0.0 10.0 drag 0.2"
    call("echo "+s+">"+fn, shell=True)
    call("time mpirun -np 2 lmp_openmpi -sf opt < "+fn, shell=True) # use optimization for pair_coeff
    s="thermo 10 >"+fn, shell=True
    call("echo "+s+">"+fn, shell=True)
    s="run 3000" # number of time step
    call("echo "+s+">"+fn, shell=True)
    call("time mpirun -np 2 lmp_openmpi -sf opt < "+fn, shell=True)
```

download: [lattice.py](#)

download: [fcc111.py](#)

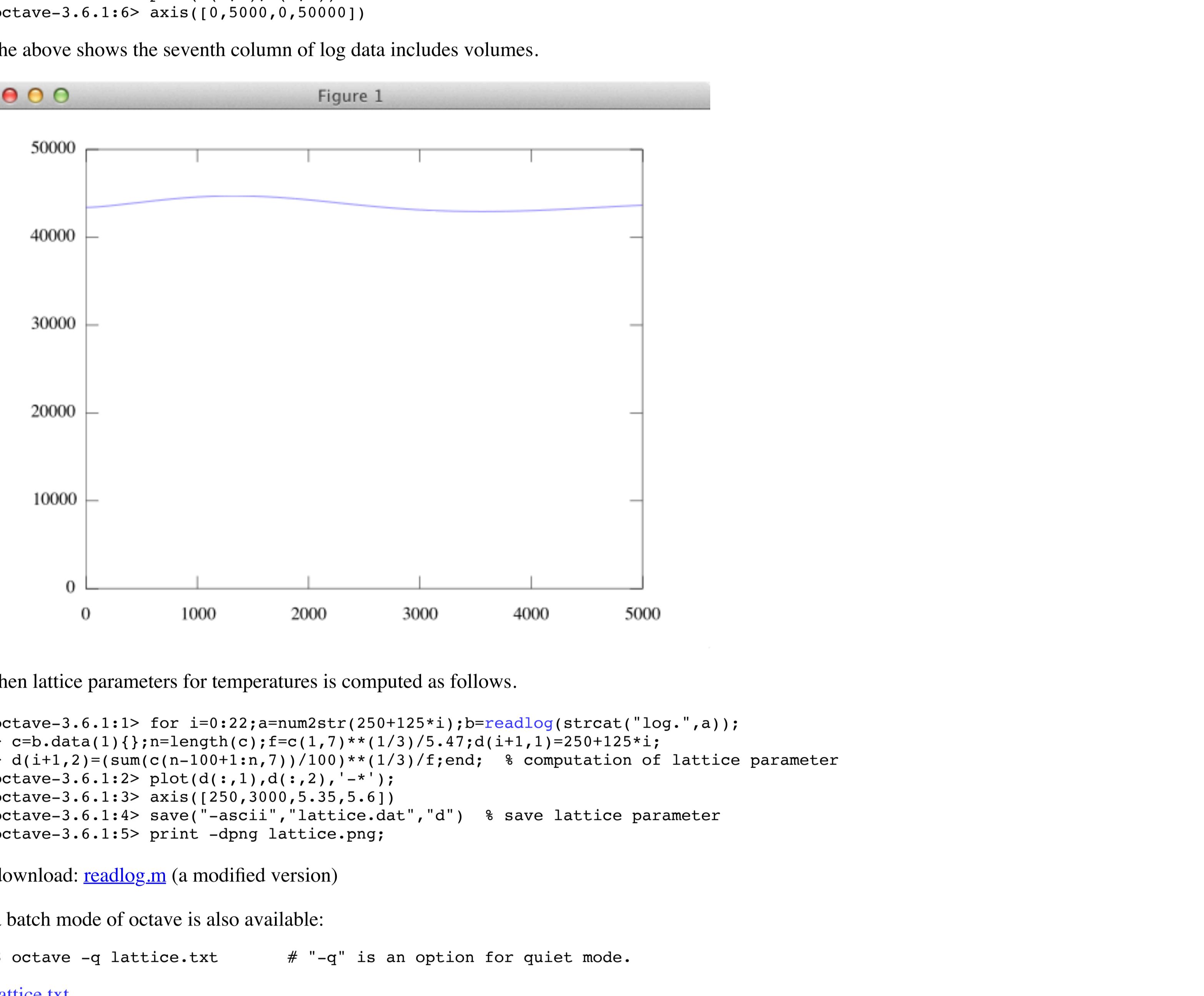
usage:

```
$ ./fcc111.py > data.fcc111
$ ./lattice.py
```



via 「黒蜜大樹 湯の枝」 「ボコ」のイラスト [pixiv] in japanese

"a big tree of black honey and a sprig of hot water" / illustration by pokot [pixiv]



via 「黒蜜大樹 湯の枝」 「ボコ」のイラスト [pixiv] in japanese

"a big tree of black honey and a sprig of hot water" / illustration by pokot [pixiv]

the computation was done from 250K to 3000K.

$UO_2$  on fcc111 lattice was employed and its system size was 3000 atoms (U=1000, O=2000).

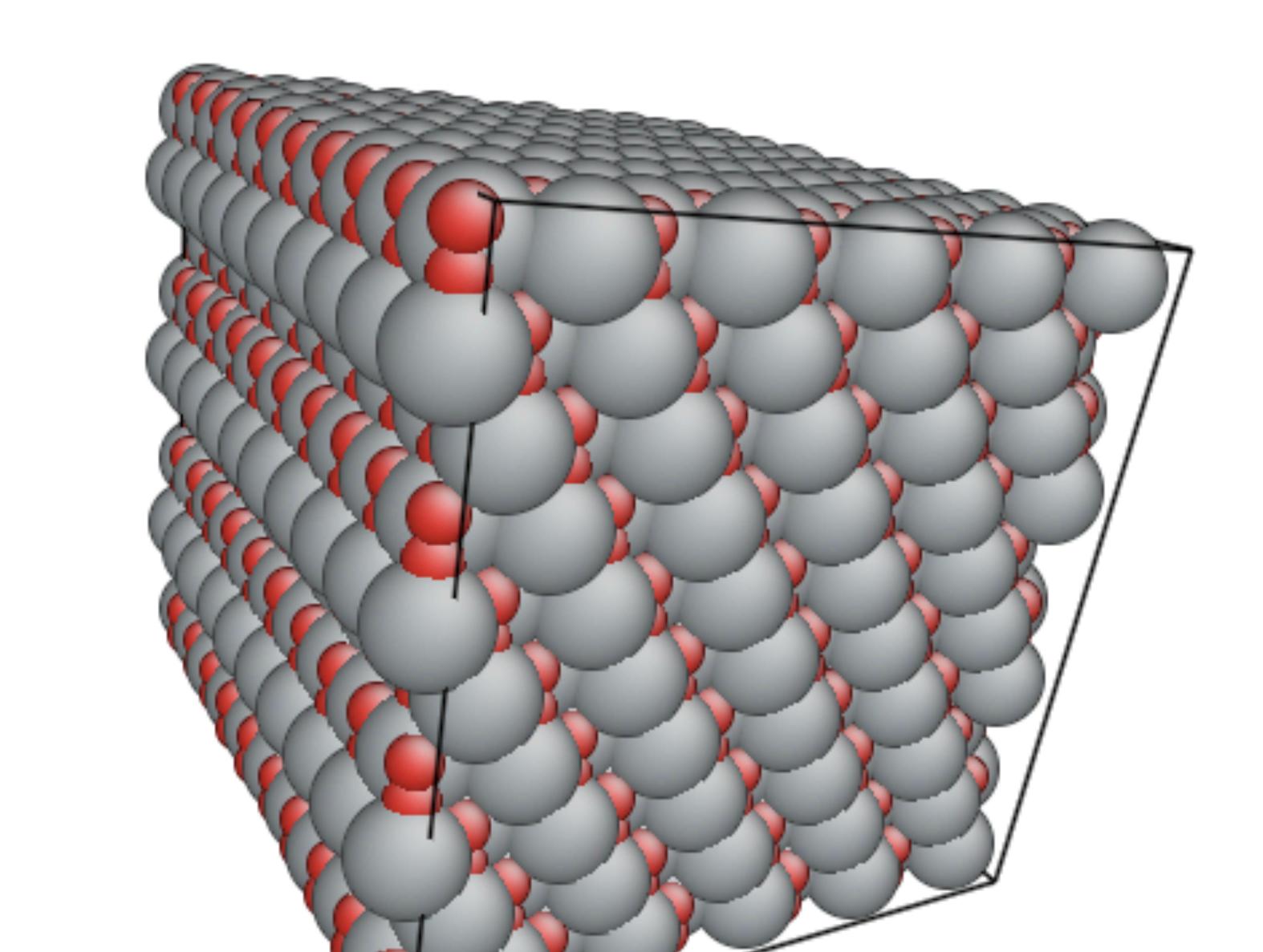
post-process with octave of lammps computation was done as follows:

```
octave-3.6.1:2> a=readlog("log.1500");
octave-3.6.1:3> a
WARNING: terminal is not fully functional
a =(press RETURN)

scalar structure containing the fields:
Chead =
{
  [1,1] = Step
  [1,2] = Temp
  [1,3] = E_pair
  [1,4] = E_mol
  [1,5] = TotEng
  [1,6] = Press
  [1,7] = Volume
  [1,8] =
}
data =
{
  [1,1] =
  0.0000e+00  1.5000e+03 -3.0472e+04  0.0000e+00 -2.9991e+04  4.7107e+05  4.3399e+04
  1.0000e+01  4.7469e+03 -3.7655e+04  0.0000e+00 -3.5815e+04  1.1936e+05  4.3400e+04
  2.0000e+01  1.3793e+03 -3.7140e+04  0.0000e+00 -3.6637e+04  1.2023e+05  4.3403e+04
  3.0000e+01  3.0126e+03 -3.8240e+04  0.0000e+00 -3.7760e+04  1.2055e+05  4.3408e+04
  4.0000e+01  2.1906e+03 -3.8609e+04  0.0000e+00 -3.7760e+04  6.6932e+04  4.3412e+04
  5.0000e+01  2.4341e+03 -3.9170e+04  0.0000e+00 -3.8226e+04  6.6184e+04  4.3418e+04
  6.0000e+01  2.1992e+03 -3.9549e+04  0.0000e+00 -3.8696e+04  6.6632e+04  4.3424e+04
  7.0000e+01  2.3105e+03 -4.0018e+04  0.0000e+00 -3.9122e+04  7.8593e+04  4.3430e+04
  8.0000e+01  2.1054e+03 -4.0356e+04  0.0000e+00 -3.9540e+04  8.4733e+04  4.3438e+04
-- less -- (f)orward (b)ack, (q)uit
octave-3.6.1:4> b=a.data(1);
octave-3.6.1:5> plot(b(:,1),b(:,7))
octave-3.6.1:6> axis([0,5000,0,50000])
```

the above shows the seventh column of log data includes volumes.

Figure 1



then lattice parameters for temperatures is computed as follows.

```
> c=b.data(1){};n=length(c);f=c(1,7)**(1/3)/5.47;d(i+1,1)=250+125*i;
```

```
> d(i+1,2)=(sum((n-100+1:n,7))/100)**(1/3)/f;end; % computation of lattice parameter
```

```
octave-3.6.1:2> plot(d(:,1),d(:,2),'-*');
octave-3.6.1:3> axis([250,3000,5,35,5.6])
```

```
octave-3.6.1:4> save("ascii","lattice.dat","d") % save lattice parameter
```

```
octave-3.6.1:5> print -dpng lattice.png;
```

download: [readlog.m](#) (a modified version)

a batch mode of octave is also available:

```
$ octave -q lattice.txt # "-q" is an option for quiet mode.
```

lattice.txt

```
for i=0:22;a=num2str(250+125*i);b=readlog(strcat("log.",a));
```

```
> c=b.data(1){};n=length(c);f=c(1,7)**(1/3)/5.47;d(i+1,1)=250+125*i;
```

```
d(i+1,2)=(sum((n-100+1:n,7))/100)**(1/3)/f;end;
```

```
octave-3.6.1:2> plot(d(:,1),d(:,2),'-*');
```

```
octave-3.6.1:3> axis([250,3000,5,35,5.6])
```

```
octave-3.6.1:4> save("ascii","lattice.dat","d")
```

```
print -dpng lattice.png;
```

download: [lattice.txt](#)

the result is represented as follows:

this fig111.py system size is set at the size of mx=ny=mz=10;" is needed.

in fig111.py, system size is set at the size of mx=ny=mz=10;" is needed.

a system of  $UO_2$ : "mx=ny=mz=10;"

links

[LAMMPS Users Manual by Sandia Corporation](#)

[CLASSICAL MOLECULAR DYNAMICS SIMULATION OF UO2 by C.B. Basak \(pdf\)](#)

[AtomEye: atomistic configuration viewer](#)

[Octave forge on sourceforge.net: Octave.app](#)

[Octave setting on OS X in this site](#)

Back

[Mail to chibaif if you have some questions or ...](#)

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http://www.chem.sci.hokudai.ac.jp/~chibaif

http://www.chem.sci.hokudai.ac.jp/~chibaif/lattice.html

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http://www.chem.sci.hokudai.ac.jp/~chibaif/lattice/lattice111.html

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