Bulk modulus

$$K_T = -V\left(\frac{\partial p}{\partial V}\right)_{NT} = \varrho\left(\frac{\partial p}{\partial \varrho}\right)_{NT}$$
$$c = \sqrt{\frac{K_T}{\varrho}}$$

Argon units

$$\sigma = 3.405\ 10^{-10}\ \mathrm{m}, \qquad \varepsilon/k_B = 119\ \mathrm{K}, \qquad m = 0.040/(6.022\ 10^{23})\ \mathrm{kg}$$

In [3]:
```
from matplotlib import use
use("nbAgg")
import numpy as np
import matplotlib.pyplot as plt
```

In [4]:
```
rho,L,kT,vir1,P1,vir2,P2,vir3,P3,vir4,P4,vir5,P5,vir6,P6 = np.genfr
omtxt('pressure3.txt',skip_header=1,unpack=True)
```

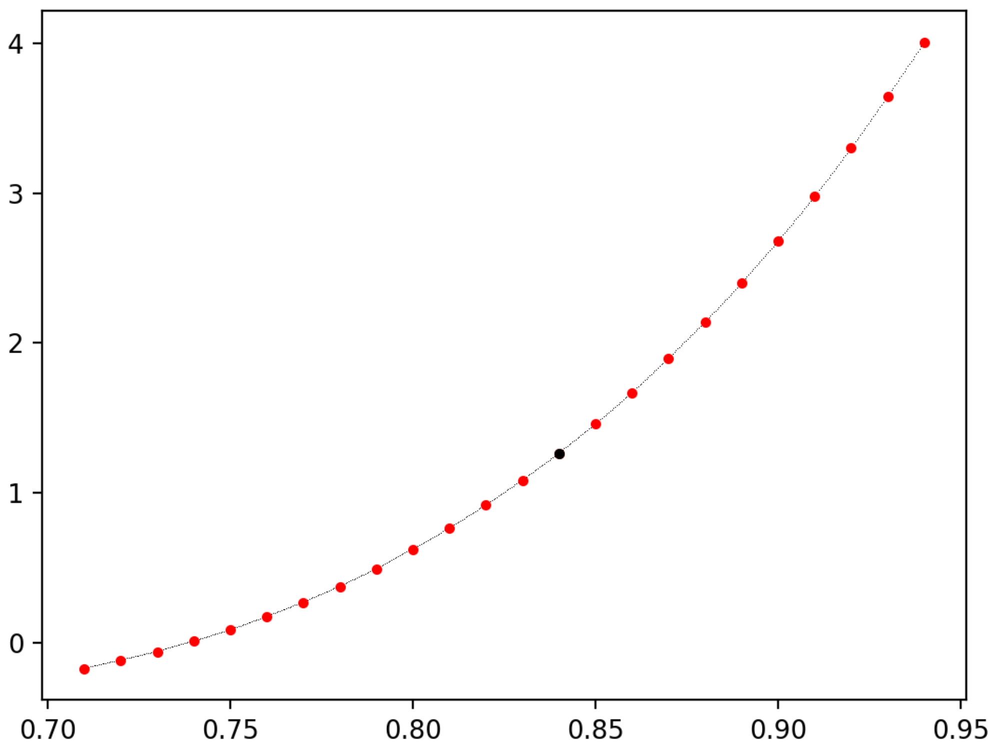
In [13]:
```
import scipy.interpolate as itp
P = (P1+P2+P3+P4+P5+P6)/6.
for i in range(np.size(L)-1,-1,-1):
    print("%3d  %12.5f  %12.5f" % (i,L[i],P[i]) )
fp = itp.interp1d(rho, P, kind='cubic')
```

```
 23      9.72290       4.00675
 22      9.75760       3.64422
 21      9.79280       3.30027
 20      9.82860       2.97572
 19      9.86480       2.67883
 18      9.90170       2.39682
 17      9.93900       2.13873
 16      9.97700       1.89670
 15     10.01550       1.66707
 14     10.05460       1.45817
 13     10.09430       1.26288
 12     10.13470       1.08235
 11     10.17580       0.91670
 10     10.21750       0.76252
  9     10.25990       0.62256
  8     10.30300       0.49162
  7     10.34680       0.37336
  6     10.39140       0.26771
  5     10.43680       0.17122
  4     10.48300       0.08282
  3     10.53000       0.00738
  2     10.57780      -0.06148
  1     10.62660      -0.12021
  0     10.67620      -0.17531
```

In [4]:
```
dens=0.84
temp=0.84
deld=0.00001
sigma=3.405e-10
epsilon=119*1.3807e-23
mass=0.040/6.0223e23
utime=np.sqrt(mass*sigma**2/epsilon)
print('units: mass=',mass,' length=',sigma,' time=',utime,' energy=
',epsilon)
print('density d=',dens,'[LJ]',dens*mass/sigma**3,'kg/m^3')
print('temperature T=',temp,'[LJ]',temp*119,'K')
K_T = dens*(fp(dens+deld)-fp(dens-deld))/(2.*deld)
print('isothermal bulk modulus K=',K_T)
c = np.sqrt(K_T/dens)
print(' sound velocity c=',c,' [LJ]  ', c*sigma/utime,' m/s')
```

```
units: mass= 6.641980638626438e-26  length= 3.405e-10  time= 2.164
924602151941e-12  energy= 1.6430329999999999e-21
densità d= 0.84 [LJ] 1413.2713097523942 kg/m^3
temepartura T= 0.84 [LJ] 99.96 K
isothermal bulk modulus K= 15.828852889682386
 sound velocity c= 4.340952946959588  [LJ]   682.7464000226659  m/
s
```

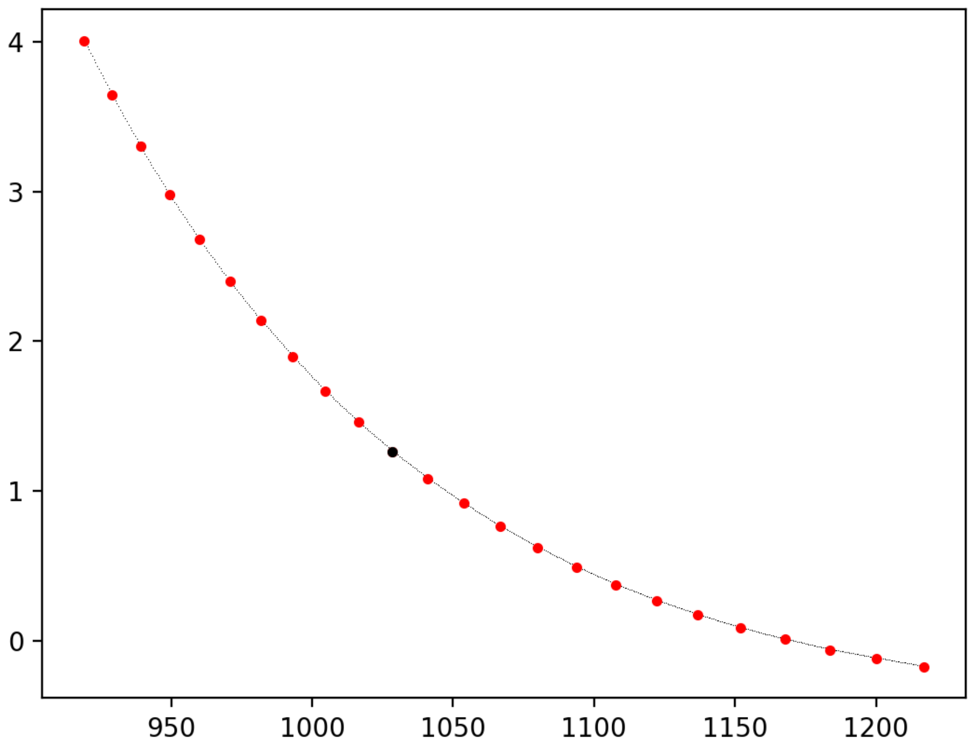
In [5]:
```
nrho = np.linspace(rho[0], rho[-1], num=512, endpoint=True)
plt.plot(nrho,fp(nrho),'k,',rho,P,'r.')
plt.plot(rho[13],P[13],'k.')
plt.savefig("rhoP.pdf")
plt.show()
```



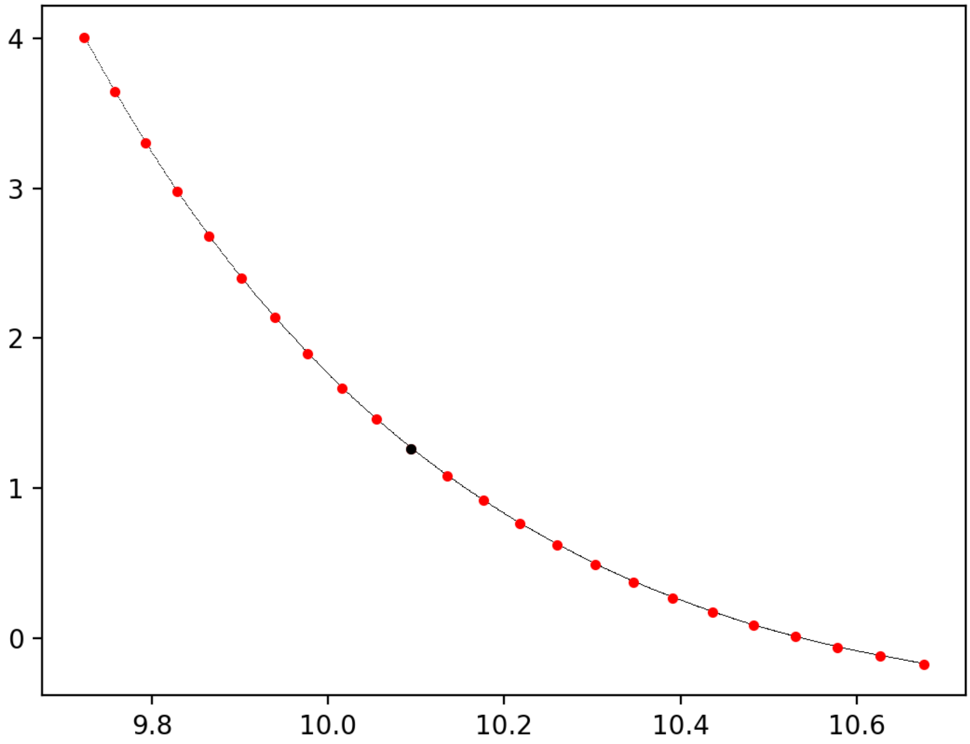
In [6]:
```
V = L**3
vol = np.linspace(L[0]**3, L[-1]**3, num=512, endpoint=True)
vp = itp.interp1d(V, P, kind='cubic')
volu=(864./0.84)
print('volume V=',volu,V[13])
temp=0.84
delv=0.1
K_T = -volu*(vp(volu+delv)-vp(volu-delv))/(2.*delv)
print('bulk modulus K_T=',K_T)
```

```
volume V= 1028.5714285714287 1028.557613261807
bulk modulus K_T= 15.83813430394278
```

In [7]:
```
V = L**3
vol = np.linspace(L[0]**3, L[-1]**3, num=512, endpoint=True)
vp = itp.interp1d(V, P, kind='cubic')
plt.plot(vol,vp(vol),'k,',V,P,'r.')
plt.plot(V[13],P[13],'k.')
plt.savefig("volP.pdf")
plt.show()
```



In [8]:
```
ell = np.linspace(L[0], L[-1], num=1024, endpoint=True)
lp = itp.interp1d(L, P, kind='cubic')
plt.plot(ell,lp(ell),'k,',L,P,'r.')
plt.plot(L[13],P[13],'k.')
plt.savefig("ellP.pdf")
plt.show()
```



In [9]:
```
0.84/(3.4**3*1e-30)*(1e-3)**3
```
Out[9]:
```
2.1371870547526967e+19
```

In [10]:
```
(0.018)**(1./3)
```
Out[10]:
```
0.2620741394208897
```

In [11]:
```
(6.022e23/(0.84/(3.4**3*1e-30)))/1e-6
```
Out[11]:
```
28.177224761904768
```

In [ ]: