```
import numpy as np
File='gen.eam.alloy'

opt_param = {'re':2.9566,'fe':1.5295,'rhoe':20.1835,'rhom':0.7073,'alpha':9.0571,'beta':5.4686,'kappa':0.4315,'lamda':0.8642,'etha':1.3071,'A':0.2129,'B':0.3136, 'Fe':-2.4240,'Fm0':-2.2719,'Fm1':-0.8405,'Fm2':1.7548,'Fm3':0.3234,'Fn0':-2.3842,'Fn1':-0.4126,'Fn2':1.0258,'Fn3':-2.9954,'F0':-2.4221,'F1':0.0000,'F2':1.8160,'F3':0.8806}

locals().update(opt_param)
(rhol,rhon,rho0)= (rhom*rhoe,0.85*rhoe,1.15*rhoe)

rho_list = np.arange(0.0,(2.0-0.2*10**(-4))*rhoe, 0.2*10**(-3)*rhoe)
r_list = np.arange(0.0, 7.0-0.7*10**(-4), 0.7*10**(-3))
F_rho_list = []
phi_r_list = []
rho_r_list = []
rphi_r_list = []

for rhoi in rho_list:
    if 0.0 <= rhoi < rhol:
        F_rho = Fm0*(rhoi/rhol -1)**0 + Fm1*(rhoi/rhol -1)**1 + Fm2*(rhoi/rhol -1)**2 + Fm3*(rhoi/rhol -1)**3
    elif rhol <= rhoi < rhon:
        F_rho = Fn0*(rhoi/rhon -1)**0 + Fn1*(rhoi/rhon -1)**1 + Fn2*(rhoi/rhon -1)**2 + Fn3*(rhoi/rhon -1)**3
    elif rhon <= rhoi <rho0:
        F_rho = F0*(rhoi/rhoe -1)**0 + F1*(rhoi/rhoe -1)**1 + F2*(rhoi/rhoe -1)**2 + F3*(rhoi/rhoe -1)**3
    elif rhoi >= rho0:
        F_rho = Fe*(1- etha*np.log(rhoi/rhoe))*(rhoi/rhoe)**etha
    F_rho_list.append(F_rho)

for r in r_list:
    phi_r = (A*np.exp(-alpha*(r/re -1)))/(1+(r/re-kappa)**20) - (B*np.exp(-beta*(r/re -1)))/(1+(r/re-lamda)**20)
    rho_r = (fe*np.exp(-beta*(r/re -1)))/(1+(r/re-lamda)**20)
    rphi_r = r*phi_r
    phi_r_list.append(phi_r)
    rho_r_list.append(rho_r)
    rphi_r_list.append(rphi_r)

```

```
35  f = open(File, 'w')
36  f.write('This is generated by Xin group. \n')
37  f.write('Au eam potential. \n')
38  f.write('Contact: hxin@vt.edu \n')
39  f.write('1 Au \n')
40  Nrho = len(rho_list)
41  drho = rho_list[1]-rho_list[0]
42  Nr = len(r_list)
43  dr = r_list[1]-r_list[0]
44  cutoff = r_list[-1]
45  f.write('%d %16e %d %16e %16e\n' % (Nrho, drho, Nr, dr, cutoff))
46
47  LattConst = re*np.sqrt(2.0)  #LattConst of FCCmetal=re*np.sqrt(2.0)
48  f.write('%d    %e    %e      %s  \n' % (79, 0.1969670000E+03,
        LattConst, 'fcc')) #atomic numbers, mass, LattConst,
        LatticeType
49
50  for i in range(Nrho):
51      f.write('%.10e\n' % F_rho_list[i])
52
53  for i in range(Nr):
54      f.write('%.10e\n' % rho_r_list[i])
55
56  for i in range(Nr):
57      f.write('%.10e\n' % rphi_r_list[i])
58
59  f.close()
```