Work conjugate strain of virial stress

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ABSTRACT

Certain stress tensor and strain tensor form a conjugate pair if there exists a scalar valued strain energy function such that the stress tensor is equal to the derivative of strain energy function with respect to the strain tensor. Virial stress is widely accepted as the stress measurement in molecular dynamics (MD). However, its conjugate strain is not yet identified. An atomic logarithmic strain is proposed and numerically verified as the conjugate strain of virial stress at 0 K temperature. The strain energy is calculated by virial stress and the proposed atomic logarithmic strain equals to the interatomic potential energy density. This conclusion is numerically verified with (1) Coulomb-Buckingham potential, Lenard-Jones potential, or arbitrary nonlinear pair potential and (2) randomly generated atomic configurations and deformation gradients. Examples are given in determining the stress–strain relation for magnesium oxide with MD simulation. The result shows that the atomic logarithmic strain is identical to engineering strain when deformation is small.

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1. Introduction

The atomic definition of stress and strain is important because it bridges the gap between molecular dynamics (MD) and continuum mechanics (CM). In the process of sequential multi-scale modeling, the information of the smaller scale is extracted and used as the input for larger-scale simulation. Problem occurs when this methodology is applied to connect MD with CM. The outputs of MD simulation are force and position of all atoms. However, the input of CM simulation requires the stress–strain relation. The connection is impossible unless the force and position can be converted to stress and strain. The atomic stress is less controversial since virial stress is widely accepted as a valid stress measurement in MD. In terms of strain definition, the story is much complex. Consider a group of atoms with one atom fixed to the coordinate origin. The relative position vectors of other atoms in their original configuration and deformed configuration are $\mathbf{A} = [A_1\ A_2\ A_3]^T$, $\mathbf{C} = [C_1\ C_2\ C_3]^T$, and $\mathbf{a} = [a_1\ a_2\ a_3]^T$, $\mathbf{b} = [b_1\ b_2\ b_3]^T$, $\mathbf{c} = [c_1\ c_2\ c_3]^T$, respectively. The deformation gradient $\mathbf{F}$ may be calculated by Equations (1)–(3).

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\[
\begin{align*}
[ a_1 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ A_1 ] \\
[ a_2 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ A_2 ] \\
[ a_3 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ A_3 ]
\end{align*}
\] (1)

\[
\begin{align*}
[ b_1 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ B_1 ] \\
[ b_2 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ B_2 ] \\
[ b_3 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ B_3 ]
\end{align*}
\] (2)

\[
\begin{align*}
[ c_1 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ C_1 ] \\
[ c_2 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ C_2 ] \\
[ c_3 ] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} [ C_3 ]
\end{align*}
\] (3)

Notice that there are nine unknowns in \( \mathbf{F} \). For a system less than four atoms, deformation gradient \( \mathbf{F} \) is not unique because there are more unknowns than equations. For a system more than four atoms, a single deformation gradient \( \mathbf{F} \) may not exist because there are more equations than unknowns.

A method was introduced [1] to calculate deformation gradient by minimizing the mapping error of a single deformation gradient for a group of atoms. Assuming a single deformation gradient exists for a group of atoms, the next question becomes ‘what is the conjugate strain corresponding to virial stress?’ In the finite deformation theory of continuum mechanics, there exist many different kinds of stresses and strains. Only certain pair of stress tensor \( \mathbf{A} \) and strain tensor \( \mathbf{B} \) are related as

\[
\mathbf{A} = \frac{\partial U}{\partial \mathbf{B}}.
\]

Upon integration \( \int \mathbf{A} \mathbf{d\mathbf{B}} \), it equals to the scalar valued strain energy function \( U \). In such case, \( \mathbf{A} \) and \( \mathbf{B} \) are named as a thermodynamic pair and said to be conjugate to each other. Choosing a conjugate pair of stress and strain in material modeling is a common practice in CM. A logarithmic strain tensor is proposed here. Such strain is numerically verified to be the conjugate strain of virial stress.

Let us first introduce a ‘logm’ function. Consider the following treatment is applied to the single deformation gradient for a group of atoms. The deformation gradient can be decomposed as

\[
\mathbf{F} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{-1}
\] (4)

where

\[
\mathbf{Q} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{v}_{11} & \mathbf{v}_{12} & \mathbf{v}_{13} \\ \mathbf{v}_{21} & \mathbf{v}_{22} & \mathbf{v}_{23} \\ \mathbf{v}_{31} & \mathbf{v}_{32} & \mathbf{v}_{33} \end{bmatrix}, \quad \mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}
\] (5)

\( \lambda_1, \lambda_2, \lambda_3 \) are the three eigenvalues of the deformation gradient; \( \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3 \) are the three corresponding eigenvectors. Notice that \( \mathbf{\Lambda} \) is a diagonal matrix, one may define

\[
\log(\mathbf{\Lambda}) = \begin{bmatrix} \log \lambda_1 & 0 & 0 \\ 0 & \log \lambda_2 & 0 \\ 0 & 0 & \log \lambda_3 \end{bmatrix}
\] (6)

An asymmetric logarithmic strain \( \hat{\mathbf{\Lambda}} \) is defined as
\[ \hat{\mathbf{L}} = \mathbf{Q} \log(\mathbf{\Lambda}) \mathbf{Q}^{-1} \] (7)

This process is identical to ‘\( \logm(\mathbf{F}) \)’ function in MATLAB®, where the matrix logarithmic is formally defined by Culver [2] and numerically programmed into MATLAB® by a method developed by Davies and Higham, Cheng, and Higham [3–5].

\[ \hat{\mathbf{L}} = \logm(\mathbf{F}) \] (8)

A symmetric logarithmic strain is defined as the symmetric part of asymmetric logarithmic strain tensor

\[ \mathbf{L} = \frac{1}{2} (\hat{\mathbf{L}} + \hat{\mathbf{L}}^T) \] (9)

The deformation gradient \( \mathbf{F} \) must satisfy the following two conditions for the conjugacy between the logarithmic strain and the virial stress to be valid:

(a) The matrix log of \( \mathbf{F} \) yields a real-valued matrix

\[ \Im \logm(\mathbf{F}) = 0 \] (10)

(b) The determinant of \( \mathbf{F} \) is positive

\[ \det(\mathbf{F}) > 0 \] (11)

When conditions (a) and (b) are satisfied, it can be analytically proved that

\[ (\logm(\mathbf{F}))^T = \logm(\mathbf{F}^T) \] (12)

Its numerical verification is presented in Appendix 1. Hence, Equation (9) becomes

\[ \mathbf{L} = \frac{1}{2} (\logm \mathbf{F} + \logm \mathbf{F}^T) \] (13)

It is numerically verified that the conjugacy remains valid for the deformation gradient \( \mathbf{F} \) that satisfied conditions (a) and (b), even if it has imaginary eigenvalues.

Also, \( \mathbf{L} \) and \( \hat{\mathbf{L}} \) are objectives (material frame indifference). The numerical verification is presented in Appendix 2 to shows that

\[ \mathbf{L} = \mathbf{Q}^T \mathbf{L}' \mathbf{Q} = \mathbf{Q}^T \frac{1}{2} \left[ \logm \mathbf{Q}^T \mathbf{F} \mathbf{Q} + \logm(\mathbf{Q}^T \mathbf{F} \mathbf{Q})^T \right] \mathbf{Q} \] (14)

\[ \hat{\mathbf{L}} = \mathbf{Q}^T \hat{\mathbf{L}}' \mathbf{Q} = \mathbf{Q}^T \frac{1}{2} (\logm \mathbf{Q}^T \mathbf{F} \mathbf{Q}) \mathbf{Q} \] (15)

Therefore, both \( \mathbf{L} \) and \( \hat{\mathbf{L}} \) are valid strain measures that can be used as independent constitutive variables in CM.

### 2. Numerical verification

Consider \( N \) atoms move from the original positions \( \mathbf{X}^n \) to the deformed positions \( \mathbf{x}^n(n = 1, 2, 3, \ldots, N) \) under a single deformation gradient \( \mathbf{F} \), where the superscript identifies the atom and the subscripts denote three degrees of freedom.
\[ X^n_j = F^n_j X^n_j \]  

Let us first calculate the total interatomic potential energy difference between the initial and the final stages. In MD simulation with pair potential, the interatomic potential energy \( U^{mn} \), between two atoms \( m \) and \( n \), is explicitly given as a function of their relative position vector

\[ r^{mn}_i = X^n_i - X^j_i \]  
\[ R^{mn}_i = X_i^n - X_i^j \]

The difference of interatomic potential between the original and the deformed stages is obtained as

\[ \Delta U = \frac{1}{2} \sum_{m=1}^{N} \sum_{n=1, n \neq m}^{N} U^{mn}(r^{mn}_i) - \frac{1}{2} \sum_{m=1}^{N} \sum_{n=1, n \neq m}^{N} U^{mn}(R^{mn}_i) \]

On the other hand, the strain energy calculation requires numerical integration. Therefore, the deformation gradient is divided into \( K \) incremental steps. The incremental deformation gradient

\[ kF_{ij} = k \left( F_{ij} - \delta_{ij} \right) + \delta_{ij}, \quad k \in \{0, 1, 2, 3, \ldots, K\} \]

The atomic logarithmic strain of each step can be calculated directly from the deformation gradient

\[ kL_{ij} = \frac{1}{2} \left( \log kF_{ij} + \log kF_{ji} \right) \]

It is seen that \( 0F_{ij} = \delta_{ij} \) and \( 0L_{ij} = 0 \). The position vector of the \( k \)-th incremental step is

\[ kX^n_i = kF_{ij} X^n_j \]
\[ X^n_j = kF_{ji}^{-1} kX^n_i \]

The virial stress at 0 K of the \( k \)-th step, \( kS_{ij} \), is calculated as

\[ kS_{ij} = \frac{1}{2V} \sum_{m=1}^{N} \sum_{n=1, n \neq m}^{N} \left( kX^m_i - kX^j_i \right) \left( kF_{ij}^{mn} \right) \]

where the interatomic force, \( f_{ij}^{mn} \), as a function of relative position is explicitly given in MD simulation.

\[ f_{ij}^{mn} = - \frac{\partial U}{\partial r_{ij}^{mn}} \]

The strain energy in its continuum form

\[ E = \int_V \int_S dL_i dV = \int_V \int \frac{1}{4} (\mathbf{x}^m - \mathbf{x}^n) \otimes (\mathbf{f}^m - \mathbf{f}^n) \log \left[ \mathbf{F} + \log \mathbf{F}^T \right] dV \]
The strain energy in its discrete form with numerical integration

\[ LE = V \sum_{k=1}^{L} \frac{1}{2} (k S + k^{-1} S) : (k L - k^{-1} L) \]

\[ = V \sum_{k=1}^{L} \sum_{m=1}^{N} \sum_{n=1,n \neq m}^{N} \frac{1}{4} \left( k S_{mn} + k^{-1} S_{mn} \right) : \left( k L_{mn} - k^{-1} L_{mn} \right) \]

\[ = V \sum_{k=1}^{L} \sum_{m=1}^{N} \sum_{n=1,n \neq m}^{N} \frac{1}{4} \left[ (k x_{m} - k x_{n}) \otimes (k f_{m} - k f_{n}) + (k^{-1} x_{m} - k^{-1} x_{n}) \otimes (k^{-1} f_{m} - k^{-1} f_{n}) \right] \]

\[ = \frac{1}{2} \left[ \logm(k F + k F^{T}) - \logm(k^{-1} F + k^{-1} F^{T}) \right] \tag{27} \]

where \( L \in \{1, 2, 3, \ldots, K\} \). It is noticed that

\[ LE = U(\tilde{L}) - U(X) \tag{28} \]

where \( \tilde{L} = \{\tilde{L}_{m}|m = 1, 2, 3, \ldots, N\} \) denotes the atomic position of the \( L \)-th loading step.

In Appendix 3, it is numerically verified that the strain energy obtained from \( E = V \int S : dL \) equals to the difference of interatomic potential energy between current state and initial state

\[ \Delta U = E \tag{29} \]

Different cases have been tested with randomly generated atom positions, electric charges, and deformation gradient. Leonard-Jones potential, Coulomb-Buckingham potential, and some artificial nonlinear spring potential are tested and the results conclude that the conjugacy is valid for all cases. In this work, the verification is restricted to pair potential. The strain energy \( E \) and interatomic potential energy \( \Delta U \) match perfectly as shown in Figure 1.

It is seen that the interatomic potential energy and the strain energy are identical at all integration steps. It is verified that the asymmetric logarithmic strain tensor \( \tilde{L} = \logm(F) \) is also the conjugate strain of virial stress. Notice that virial stress is symmetric by definition. In Equation (26), only the symmetric part of the logarithmic strain tensor contributed to the integration.

\[ E = \int_{V} S_{ij} dL_{ij} dV = \int_{V} S_{ij} d(\tilde{L}_{ij} - \tilde{L}_{ij}) dV = \int_{V} S_{ij} d\tilde{L}_{ij} dV \tag{30} \]

where \( \tilde{L}_{ij} \) is the antisymmetric part of the asymmetric atomic logarithmic strain \( \tilde{L}_{ij} \), that is,

\[ \tilde{L} = L + \tilde{L} \tag{31} \]

Therefore,

\[ U = \int_{V} S_{ij} d\tilde{L}_{ij} dV \tag{32} \]
3. Examples of MD simulation

Utilizing the atomic logarithmic strain, an MD simulation is conducted to calculate stress–strain relation of a single crystal magnesium oxide. Magnesium oxide is simulated with Coulomb-Buckingham potential. The specimen is placed along \( \langle 100 \rangle \) direction with one end fixed, that is, \( u_y(y = 0) = 0 \) and the other end, at \( y = l \), free. The kinetic energy was damped out and the specimen reached steady state at 0 K. This configuration is considered as the original stage \( X_0 \) for strain calculation. The artificial damping is then removed and the free end is slowly pulled upward along \( y \)-direction with a displacement specified boundary condition. The stress and strain are calculated for each unit cell and the average value of eight unit cells are recorded for the purpose of display. This process is similar to the calculation of element center value based on the nodal values in finite element analysis. In principle, a single deformation gradient may not exist for a group of atoms more than four. An optimization process suggested by Gullett et al. [1] is utilized to find the optimized deformation gradient that best describes the atomic motion. This deformation gradient is then utilized to calculate the atomic logarithmic strain. LAPACK [6], an open-source FORTRAN library, is used for eigenvalue and eigenvector calculation. For convenience, Tecplot® is utilized to present the simulation result. The position of each node is calculated through the average location of eight atoms in a unit cell. The stress and strain values of each element come from the average of its eight nodes.

Figure 1. Comparison between strain energy and interatomic potential energy of four deformation gradients.
Although the equivalent of atomic logarithmic strain in CM is not identified yet (the same is true for the virial stress, unfortunately), as a finite strain measurement, atomic logarithmic strain should be close to elongation, $e = (y - y_0)/y_0$ when the deformation is small. Here, $y_0$ is the original length of specimen, and $y$ is the deformed length of the specimen. Indeed, this predication is observed in Figures 3(a) and 2(b), and also in Figure 4. It should be emphasized that the problem presented here is not a so-called ‘Simple Problem’ in CM; in other words, the strain and the stress are not at all uniform throughout the specimen after necking. This is evidenced by the distribution of the logarithmic strain (the $L_{22}$ component) in the whole specimen as shown in Figure 2(c)–(f). The stress–strain relation of magnesium oxide at 0 K indicated by virial stress $S_{22}$ versus the atomic logarithmic strain $L_{22}$ is shown in Figure 3. It is noticed that the stress–strain curve is quite smooth from stage (a) to stage (c) as marked in Figure 2. The atomic logarithmic strain $L_{22}$ versus elongation is shown in Figure 4. One may clearly see that the curve (red color) becomes a straight line (blue color) before necking occurs. It is also remarked that the virial stress and the atomic logarithmic strain presented in Figures 3 and 4 are probed at the node marked by ‘X’ in Figure 2.

4. Discussion

The conjugacy between the virial stress and the atomic logarithmic strain hinges on the requirement that a uniform deformation gradient exists for all atoms involved in the virial stress calculation. Those atoms outside of the cut-off distance have no contribution to the calculation of virial stress of a group of atoms; hence, the deformation gradient of those outside atoms is irrelevant. Practically, most interatomic potentials have a cut-off ranging from one lattice constant to less than a hundred lattice constants, and it is reasonable to assume a single deformation gradient exists for the atoms within the cut-off.
Hencky strain $\mathbf{h}$ [7–9] in CM is defined based on the logarithm of deformation gradient after polar decomposition [3,10,11], that is,

$$\mathbf{F} = \mathbf{RU} = \mathbf{VR}$$  \hspace{1cm} (33)

$$\mathbf{h} = \logm(\mathbf{V})$$  \hspace{1cm} (34)

We have numerically verified that such strain, $\mathbf{h}$, is not the conjugate to virial stress. The conjugacy to virial stress is not guaranteed if the polar decomposition is carried out and ‘logm’ operates on $\mathbf{V}$. The reason is that the stress and strain are summated from the values calculated by many atoms in MD simulation; such operation requires that the tensor has the same base for the summation to be meaningful. The tensors of different bases cannot be added together. If the rigid body rotation is removed from the deformation gradient before the ‘logm’ operation, the calculated strain tensor loses all

\[ \text{Figure 3. Stress–strain relation of magnesium oxide single crystal at 0 K at } <100> \text{ direction.} \]

\[ \text{Figure 4. Relationship between atomic logarithmic strain } (L_{22}) \text{ and elongation } ((y - y_o)/y_o). \]
the information about its original coordinate, preventing it from adding to another tensor from other atoms with different base and different rigid body rotation.

It would be interesting to investigate the corresponding continuum counterpart of virial stress. It is known that Kirchhoff stress is the conjugate stress of Hencky strain in CM [7–9]. We have verified that the atomic logarithmic strain is different from Hencky strain. In fact, the form of atomic logarithmic strain is different from any known strain definitions. The next goal is to rigorously define various kinds of stresses and strains in MD with their counterparts in CM identified. With the completion of such effort, it is then possible to derive stress–strain relation based on MD simulation.

Disclosure statement
No potential conflict of interest was reported by the authors.

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Appendix 1. MATLAB® code to verify \((\logm F)^T - \logm(F^T)\)

The following is the code. One may run the code with MATLAB and the result shows that \((\logm F)^T - \logm(F^T) \approx 0\).

```matlab
clear
clc
F = rand(3,3)
logm(F') - logm(F)
```

Appendix 2. MATLAB® code to verify the objectivity of \(L\) and \(\dot{L}\)

The following is the code. One may run the code with MATLAB and verify that Equations (14) and (15) are satisfied.

```matlab
clear
clc
F=rand(3,3); %random 3X3 deformation gradient
alpha=rand;  %rotational angle about x axis
beta=rand;   %rotational angle about y axis
gamma=rand;  %rotational angle about z axis
Rx=[ 1 0 0; 0 cos(alpha) -sin(alpha); 0 sin(alpha) cos(alpha)];
Ry=[ cos(beta) 0 sin(beta); 0 1 0; -sin(beta) 0 cos(beta)];
Rz=[ cos(gamma) -sin(gamma) 0; sin(gamma) cos(gamma) 0; 0 0 1];
dcm=Rx*Ry*Rz; FF=dcm'*F*dcm;
D=logm(F);
DD=logm(FF);
'Asymmetric Atomic Logarithmic Strain is objective if value==0'
dcm'*D*dcm-DD
A=zeros(3,3);
AA=zeros(3,3);
for i=1:3
    for j=1:3
        A(i,j)=1/2*(D(i,j)+D(j,i));
        AA(i,j)=1/2*(DD(i,j)+DD(j,i));
    end
end
'Symetric Atomic Logarithmic Strain is objective if value ==0'
dcm'*A*dcm-AA
```
Appendix 3. MATLAB® code to verify that atomic logarithmic strain and viral stress are a conjugate pair in molecular dynamics

The following is the code. One may run the code with MATLAB and the result shows that atomic logarithmic strain and viral stress are a conjugate pair in molecular dynamics and, upon integration, the strain energy equals to the interatomic potential energy.

clear
clc

close all

% This is the program that numerically proved that the conjugate
% strain of virial stress is atomic logarithmic strain.
% The stress is the classical virial stress defined on a group
% of atoms. The strain is calculated from a single
% displacement gradient for all atoms.
% The matrix log is performed on the
% deformation gradient and symmetric part of the result strain
% matrix is the atomic logarithmic strain

% Written by Leyu Wang. 08/21/2015.
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% associated paper is published.

% variable declarations

dstep=177 % 177 numerical integration steps
X=randn(3,7) % coordinate of 7 undeformed atoms (random)
q=randn(1,7) % electric charge of 7 atoms (random)

for i=1:1:length(q)
    if q(i)>(1/2)
        q(i)=1
    else
        q(i)=-1
    end
end

A=0.3 % Coulomb-Buckingham Potential Parameter
B=0.2 % Coulomb-Buckingham Potential Parameter
C=0.5 % Coulomb-Buckingham Potential Parameter
e=0.15 % Coulomb-Buckingham Potential Parameter

anum=max(size(X)) % total number of atoms

epsl=0.15 % Coulomb-Buckingham parameter
sigma=0.12 % Coulomb-Buckingham parameter
volume=1.2 % Volume of unit cell

x=zeros(3,anum) % coordinate of the deformed atoms
r=zeros(3) % relative potions vector of each j atom
% regards to an i atom

rs=0 % scalar value of r
f=zeros(3,1)  \% force vector of each j atom regards to a
    \% specific i atom
fs=0  \% scalar value of f
strain=zeros(3,3) \% "atomic logarithmic" strain
laststrain=zeros(3,3) \% "atomic logarithmic" strain of last
    \% deformation step
laststress=zeros(3,3) \% virial stress of last deformation step
AA=zeros(3,3)
BB=zeros(3,3)
StrainE=zeros(1,dstep) \% "atomic logarithmic" strain of each
    \% integration step
PotentialE=zeros(1,dstep) \% Potential energy of each integration
    \% step
V=0  \% Interatomic Potential Energy (absolute value)
ECM=0  \% Strain Energy (absolute value)
ct=0  \% logical control switch
FA=zeros(3,3) \% deformation gradient
\% Randomly generate a deformation gradient FA which satisfy:
\% (I) \logm(FA) has real value \% (II) \det(FA) > 0
test=1e20
F=rand(3,3)
[aa bb]=eig(F)
\% Calculate Interatomic Potential, Stress and Strain
\% for c=0:1/dstep:1 \% c is the scale factor range from 0-1 to
ct=ct+1  \% scale FA
\% deformation gradient FA of current integration step
FA=(F-[1 0 0;0 1 0;0 0 1])*c+[1 0 0;0 1 0;0 0 1];
\% calculate current coordinate of nodes
for i=1:1:anum
    x(:,i)=FA*X(:,i)
end
\% calculate stress and strain
V=0
ctt=0
stress=0
strain=0
for i=1:1:anum
    for j=1:1:anum
if i~=j
    % Calculate relative position vector r
    ctt=ctt+1;
    r=x(:,i)-x(:,j);
    rs=norm(r);
    % Leonard Johns Force
    fs=4.*eps1.*(-12.*sigma.^12.*rs.^(-13)+6.*sigma.^6.*rs.^(-7))
    % Buckingham force
    fs=(6.*c)/rs^7 - (A*B)/exp(B*rs) - (q(i)*q(j))/(2*pi*e*rs^2);
    ff=fs.*r./norm(r);
    % virial stress of O-K (defined on a group of atoms)
    stress=stress+ff'/2/volume;
    % Leonard Johns Potential
    V=V+ (4.*eps1.*sigma.^12.*rs.^(-12)-sigma.^6.*rs.^(-6))./2;
    % Column Buckingham Potential
    V=V+(A/exp(B*rs) - C/rs^6 + (q(i)*q(j))/(2*pi*e*rs^2))/2;
    % atomic logarithmic strain (No polar decomposition before logm)
    AA=logm(AF)/((aum-1)/aum);
    % keep only the symmetric part of logm(AF)
    for ii=1:3
        for jj=1:3
            BB(ii,jj)=1/2*(AA(ii,jj)+AA(jj,ii));
        end
    end
    strain=strain+BB;
end
end

% Calculate strain energy by numerical integration
% for a=1:3
% for b=1:3
ECM=ECM+1/2*(stress(a,b)+laststress(a,b))*(strain(a,b)-laststrain(a,b));
end
end

% save the initial strain energy and interatomic potential energy
if ct==1
    ECM0=ECM;
    EMD0=V;
end
laststress=stress;
laststrain=strain;
StrainE(ct)=(ECM-ECM0)*volume;% Relative strain energy by subtract the value of 1st step
PotentialE(ct)=V-EMD0;% Relative interatomic potential energy by subtract the value of 0th step
end

% plot relative interatomic potential and relative strain energy of each integration step
figure (2)
hold on
tt=num2str(F);
tt=[' ',tt(1,:);';F= ',tt(2,:);',',tt(3,:)]
title(tt)
plot(real(StrainE),'mo','MarkerSize',7)
plot(PotentialE,'b+','MarkerSize',7)
legend('Strain Energy by Numerical Integration','Interatomic Potential Energy','Location','Best')
xlabel('Integration step')
ylabel('Energy (Atomic Unit) ')