

The High Performance Computing Application- The Mechanical and Thermodynamics Properties Computing through Material Simulations

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Abstract

The classical continuum mechanics is proved to succeed in many mechanics related regions where the material would deform like solid mechanics and fluid mechanics. Classical continuum mechanics simplifies the analysis of deformable material through a series of assumptions and linearizing processes, such as setting the material homogenous (the density ρ and other mechanical properties independent of location), isotropic (resulting in the symmetry of the mechanical properties), and the infinitesimal strain (linearizing the analysis), e.t.c¹.

However, under some conditions, the assumptions above could not be valid and the non-linear terms appear. For example, when the deformation is too large, the infinitesimal strain assumption fails and the material derivative no longer equals to the spatial derivative. Further more, the general practical material is not always that homogeneous as we would like it to be, so the density ρ may not be a constant and its dependence on location has to be taken into consideration.

The molecular dynamics(MD) method, however, could help us save the effort to distinguish whether the simplified assumptions valid or invalid because of the fact that we start the analysis from the scale of the physical composition of materials.

In the present work, we would go through the conservation laws of energy from the thermodynamics, since it is the rule material in nature has to follow no matter how small it is. We would combine the thermodynamic properties derived from MD as ensemble and the existing relations between elasticity and thermodynamic properties such as *internal energy* and *free energy* to finally derive the mechanical properties.

¹"Classical and Computational Solid Mechanics", by Y.C.Fung and Pin Tong, 2001, World Scientific

1 The Literature Review: Deriving Mechanical Properties from MD

All those non-ideal condition such like inhomogeneity and the large deformation compared to the size of materials would lead our analysis to the non-linear field theory, and sometimes it is beyond our ability to derive the behaviour of material under deformation. The molecular dynamics(MD), however, could be used to examine whether the simplifying assumptions could be applied.

Since general material could be regarded as the composition of atoms and molecules, and the macroscopic properties could be derived form the ensemble properties, it is reasonable to analyze the behavior of the material starting from MD.

Some trial has been conducted, such as the study of mechanical properties of copper using effective-medium theory(EMT) and MD². Its main point is that the EMT could describe the interactions between copper atoms better than the pair potential such as Lennard-Jones potentials.

Another trial is the iterative-like method of Lili Zhang, John Jasa, George Gazonas, Antoine Jerusalem, and Mehrdad Negahban.³ They assume a classical continuum mechanics-like deformation and Cauchy-stress-like stress to exist, compute the two physical value in a iterative-like way until they are matched with the ones from classical continuum mechanics way, and eventually claim that the assumed ones the exact values they want.

Also, the method combining micro-continuum theory and MD given by R.Maranganti and P.Sharma⁴ also suggests an interesting possible way through which we derive the micro-continuum properties first, and then expand the length scale to reach the ones of macro-continuum mechanics.

Although many trials have been done, the straightforward way to start from computing the thermodynamic properties such as the *free energy* and *internal energy* is from MD and combine it with the classical continuum mechanics is seldom mentioned.

The main goal of the present work is to derive a general method starting from the thermodynamics based on molecule scale simulations, combining it with the linear, homogenous, and isotropic elasticity for simplifying the analysis and effort paid to examine the results, since under such conditions, there only exists two independent variables to check: the first Lamé constant λ and the second Lamé constant μ .

²"Molecular-dynamics study of mechanical properties of copper", by P. Heino, H.Hakkinen, and K.Kaski, 1997

³"Extracting continuum-like deformation and stress from molecular dynamics simulation", by Lili Zhang, John Jasa, George Gazonas, Antoine Jerusalem, Mehrdad Negahban, 2014

⁴"A novel atomistic approach to determine strain-gradient elasticity constants: Tabulation and comparison for various metals, semiconductors, silica, polymers and the (Ir) relevance for nanotechnologies", by R.Maranganti and P.Sharma, 2007

2 The Thermodynamics and The Elasticity

2.1 The Classical Form of Relation between Thermodynamics Properties and Elasticity

For the Energy Equations of elasticity, we have:

The kinetic energy K :

$$K \equiv \int_V \frac{1}{2} \rho v_i v_i dV \quad (1)$$

where ρ is the density of material (here we assume it is independent of location), v_i is the velocity of particle in tensor form and V is the volume domain of interest.

The internal energy E :

$$E \equiv \int_V \rho \mathcal{E} dV \quad (2)$$

where \mathcal{E} is the internal energy per unit mass.

The heat input \dot{Q} :

$$\dot{Q} \equiv - \int_S h_i n_i da = - \int_V h_{i,i} dV \quad (3)$$

where h_i is the heat flux going through the surface S , da is the surface element, and n_i is the normal vector of surface element da .

The power external force exerted on the system P is:

$$\begin{aligned} P &\equiv \int_V F_i v_i dV + \int_S T_i v_i da \\ &= \int_V F_i v_i dV + \int_S (\sigma_{ij} n_j) v_i da \\ &= \int_V F_i dV + \int_V (\sigma_{ij} v_i)_{,j} dV \\ &= \int_V (F_i v_i + \sigma_{ij,j} v_i + \sigma_{ij} v_{i,j}) dV \end{aligned} \quad (4)$$

where F_i is the external force per unit volume, T_i is the traction exerting on the surface, σ_{ij} is the Cauchy stress related to the traction T_i ($T_i = \sigma_{ij} n_j$).

using the first law of thermodynamics:

$$\dot{K} + \dot{E} = \dot{Q} + P \quad (5)$$

then:

$$\begin{aligned} &\frac{1}{2} \rho \frac{D(v_i v_i)}{Dt} + \frac{1}{2} (v_i v_i) \frac{D\rho}{Dt} + \frac{1}{2} (v_i v_i) \rho v_{j,j} + \rho \frac{D\mathcal{E}}{Dt} + \mathcal{E} \frac{D\rho}{Dt} + \mathcal{E} \rho v_{j,j} \\ &= -h_{j,j} + F_i v_i + \sigma_{j,j} v_i + \sigma_{ij} v_{i,j} \end{aligned} \quad (6)$$

through continuity equations:

$$\begin{cases} \frac{D\rho}{Dt} + \rho v_{j,j} = 0 \\ \rho \frac{Dv_i}{Dt} = \sigma_{ij,j} + F_i \end{cases} \quad (7)$$

then:

$$\rho \frac{D\mathcal{E}}{Dt} = -h_{j,j} + \sigma_{ij} : \frac{1}{2}(v_{i,j} + v_{j,i}) \quad (8)$$

Consider the small neighborhood near the thermal equilibrium and the infinitesimal strain imposed very slowly:

$$\rho d\mathcal{E} = dQ + \sigma_{ij} de_{ij} \quad (9)$$

where $e_{ij} \equiv \frac{1}{2}(u_{i,j} + u_{j,i})$ and u_i is the displacement field.

Now apply the second law of thermodynamics:

$$dS = dS_e + dS_i, \quad (10)$$

where $dS_e = \frac{dQ}{T}$, dS is the increase of entropy in the system, dS_e is the increase of entropy through interaction with surroundings, dS_i is the increase entropy change occurs inside the system.

Assume it a reversible process, i.e. $d_i S = 0$, then:

$$d\mathcal{E} = T dS_m + \frac{1}{\rho} \sigma_{ij} de_{ij} \quad (11)$$

where $dQ = T \rho dS_m$ and dS_m is the specific entropy (entropy per unit mass).

Now we can define the *the strain energy function* W such that $\frac{\partial W}{\partial e_{ij}} = \sigma_{ij}$.

First, we introduce the internal energy in an isentropic process:

$$\begin{aligned} d\mathcal{E} &= T dS_m + \frac{1}{\rho} \sigma_{ij} de_{ij} \\ &= \left(\frac{\partial \mathcal{E}}{\partial S_m} \right) dS_m + \left(\frac{\partial \mathcal{E}}{\partial e_{ij}} \right) de_{ij} \end{aligned} \quad (12)$$

then:

$$\begin{cases} \sigma_{ij} = \rho \left(\frac{\partial \mathcal{E}}{\partial e_{ij}} \right) \\ T = \frac{\partial \mathcal{E}}{\partial S_m} \end{cases} \quad (13)$$

here we assume the density ρ a constant because the infinitesimal deformation is applied slowly.

Second, we introduce the *Helmholtz's free energy function* \mathcal{F} for isothermal process (T is constant):

$$\mathcal{F} \equiv \mathcal{E} - T S_m \quad (14)$$

then:

$$\begin{aligned}
d\mathcal{F} &\equiv d\mathcal{E} - d(T\mathcal{S}_m) \\
&= Td\mathcal{S}_m + \frac{1}{\rho}\sigma_{ij}de_{ij} - Td\mathcal{S}_m - \mathcal{S}_m dT \\
&= -\mathcal{S}_m dT + \frac{1}{\rho}\sigma_{ij}de_{ij} \\
&= \left(\frac{\partial\mathcal{F}}{\partial T}\right) dT + \left(\frac{\partial\mathcal{F}}{\partial e_{ij}}\right) de_{ij}
\end{aligned} \tag{15}$$

then:

$$\begin{cases} \sigma_{ij} = \rho \left(\frac{\partial\mathcal{F}}{\partial e_{ij}}\right) \\ -\mathcal{S}_m = \frac{\partial\mathcal{F}}{\partial T} \end{cases} \tag{16}$$

This is the *Helmholtz's free energy function*-stress relation in the isothermal process.

internal energy \mathcal{E}	Helmholtz's free energy \mathcal{F}
$\sigma_{ij} = \rho \left(\frac{\partial\mathcal{E}}{\partial e_{ij}}\right)$	$\sigma_{ij} = \rho \left(\frac{\partial\mathcal{F}}{\partial e_{ij}}\right)$
$T = \frac{\mathcal{E}}{\partial\mathcal{S}_m}$	$\mathcal{S}_m = -\frac{\partial\mathcal{F}}{\partial T}$

Table 1: The Comparison between the internal energy-stress relation and the free energy-stress relation

Table above is the comparison between the free energy under isothermal process and internal energy under isentropic process and the *strain energy function* W could be defined as:

$$W \equiv \rho\mathcal{E} \tag{17}$$

or:

$$W \equiv \rho\mathcal{F} \tag{18}$$

the form of *strain energy function* depends on the thermal process introduced.

Although the relations derived above seems straightforward and the results are pleasingly simple in the first glimpse, there exists some unreasonable make-up-like trick and vague part if we have a deep insight of the interior into the definitions on every term.

2.2 The Deeper Insight into The Procedure

As mentioned in the last paragraph, there exists some vague parts needing some more discussion:

1. The definition of "particle":

In most textbooks of continuum mechanics or solid mechanics, when it comes to the element composition of material, the "particle" is usually simply mentioned and defined vaguely as a part of the material of interest. It seems not a big issue when the focus is on the behaviour under the length scale of macro-continuum. However, in the time being we want to look deeply into the interior and compute the elasticity properties through thermodynamics, so we have to find out a more rigorous interpretation of "particle".

2. The "velocity" related to the body and surface element:

The power in which body force F_i exerts on the "particle" and the traction T_i exerts on the surface element da in equation-4 raises some questions: why the velocities of body element and surface element are regarded as the same? It seems more reasonable to separate the two parts apart and discuss respectively.

3. The formulation of kinetic energy(equation-1):

According to the last two items discussed above, the kinetic energy is no longer only dependent on one velocity and one density. At least, we have to separate it into two parts: the body and the surface.

Due to the reasons mentioned above, it is necessary to make some postulates and modify the derivation from the last subsection:

1. The definition of particle:

Since we want to start from the molecular dynamics to get the macro-continuum properties, basically we might postulate the "particles" to be the "molecules"(or in the case of metal: atoms) as the smallest unit which compose the material.

2. The kinetic energy :

$$K_m \equiv \int_{V_1} \frac{1}{2} \rho^B v_i^B v_i^B dV + \int_{V_2} \frac{1}{2} \rho^S v_i^S v_i^S dV \quad (19)$$

The superscript B stands for the part deeply inside the "body" in the material and S stands for the "surface" part in the point of view of classical continuum mechanics but now we consider it as another volume region, since we want to derive the kinetic energy starting from the scale of molecule.

3. The power :

The original power in which body force F_i and traction T_i exert on the material is accompanied with the same "velocity" and finally result in the last form of the equation-8 through continuity equations.

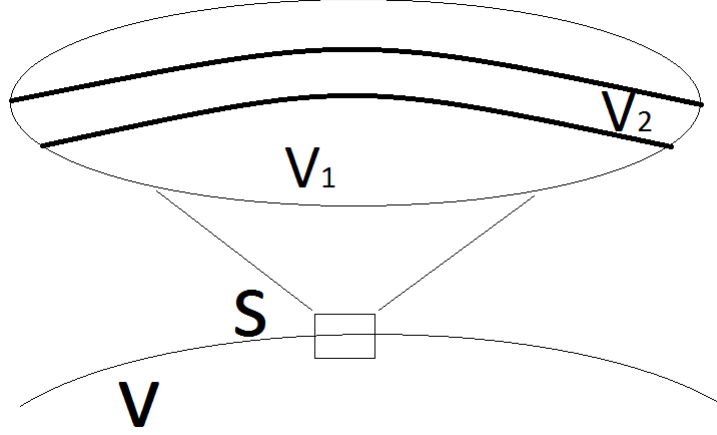


Figure 1: The scheme of the modified kinetic energy. V is the body volume and S the surface in the classical continuum mechanics. V_1 is the counterpart of V and V_2 is the one of S

Now we want to modify it into a separated form of V_1 and V_2 :

$$\begin{aligned}
P_m &\equiv \int_{V_1} F_i v_i^B dV + \int_S T_i v_i^S da \\
&= \int_{V_1} F_i v_i^B dV + \int_S (\sigma_{ij} n_j) v_i^S da \\
&= \int_{V_1} F_i v_i^B dV + \int_{V_2} (\sigma_{ij} v_i^S)_{,j} dV
\end{aligned} \tag{20}$$

Then apply the first law of thermodynamics: $\dot{K}_m + \dot{E} = P_m + \dot{Q}$ and derive the condition similar to equation-6 in the same manner :

$$\begin{aligned}
&\frac{1}{2}\rho \frac{D(v_i^B v_i^B)}{Dt} + \frac{1}{2}(v_i^B v_i^B) \frac{D\rho}{Dt} + \frac{1}{2}(v_i^B v_i^B) \rho v_{j,j}^B \\
&+ \frac{1}{2}\rho \frac{D(v_i^S v_i^S)}{Dt} + \frac{1}{2}(v_i^S v_i^S) \frac{D\rho}{Dt} + \frac{1}{2}(v_i^S v_i^S) \rho v_{j,j}^S \\
&+ \rho \frac{D\mathcal{E}}{Dt} + \mathcal{E} \frac{D\rho}{Dt} + \mathcal{E} \rho v_{j,j} \\
&= F_i v_i^B |_{V_1} + (\sigma_{ij,j} v_i^S + \sigma_{ij} v_{i,j}^S) |_{V_2} - h_{j,j}
\end{aligned} \tag{21}$$

And since:

$$\frac{1}{2}\rho \frac{D(v_i^B v_i^B)}{Dt} = v_i^B \rho \frac{Dv_i^B}{Dt} = [F_i v_i^B + \sigma_{ij,j} v_i^B] |_{V_1} \tag{22}$$

$$\frac{1}{2}\rho \frac{D(v_i^S v_i^S)}{Dt} = v_i^S \rho \frac{Dv_i^S}{Dt} = [F_i v_i^S + \sigma_{ij,j} v_i^S] \Big|_{V_2} \quad (23)$$

then:

$$\rho \frac{D\mathcal{E}}{Dt} = [-F_i v_i^S + \sigma_{ij} v_{i,j}^S] \Big|_{V_2} - \sigma_{ij,j} v_i^B \Big|_{V_1} - h_{j,j} \quad (24)$$

We put the slowly-imposed strain conditions like equation-9:

$$\rho d\mathcal{E} = (F_i du_i^S + \sigma_{ij} de_{ij}^S) \Big|_{V_2} - \sigma_{ij,j} du_i^B \Big|_{V_1} + dQ \quad (25)$$

3 The Derivation of Elasticity Properties

To derive the elastic properties, we plan to go through the following procedures:

1. Induce deformation:

In the gauge section, we have the material undergoing a deformation from the zero-state in the specified direction, compute the change of internal energy, and make the derivative of it to obtain the corresponding stress.

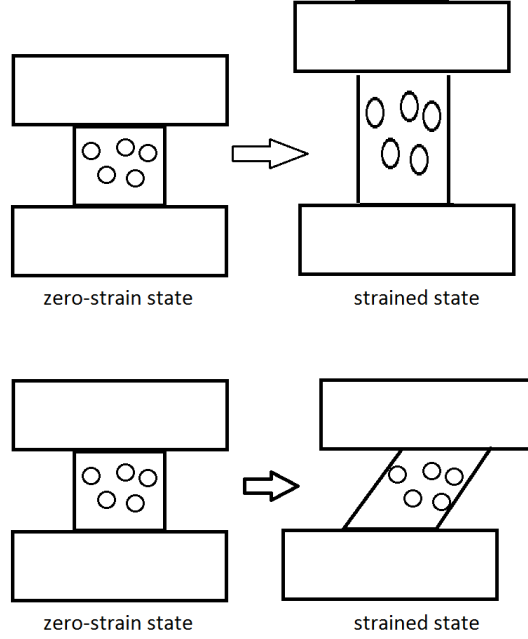


Figure 2: The deformation from the zero-strain state to the strained state in different directions.

2. Derive the Elasticity Properties:

With the strain we obtain through the set deformation and the stress we get from the internal energy derivative in the specified direction, we could eventually get the elasticity modulus C_{ijkl} :

$$\sigma_{ij} = C_{ijkl}e_{kl} \tag{26}$$

Here we only show the linear form of the elasticity modulus.

4 Example: The Linear, homogeneous, and Isotropic Material Properties Computing

In this section, we plan to derive the case of linear, homogeneous, and isotropic elasticity properties since:

1. Fewer independent variables:

In such case, there only exist two independent variables: the first Lamé constant λ and the second Lamé constant μ , and we could examine all other properties through them.

	E	ν	K
	Young's modulus	Poisson ratio	bulk modulus
μ, λ	$\frac{\mu(3\lambda+2\mu)}{\lambda+\mu}$	$\frac{\lambda}{2(\lambda+\mu)}$	$\frac{3\lambda+2\mu}{3}$

Table 2: The elasticity properties under the assumption of linear, homogenous, and isotropic material.

2. Preparing for the anisotropic case:

Thanks to the isotropic assumption helping us check the thermodynamics method work well, we could be safe to go further to the anisotropic case.

4.1 The Material Selected: Tungsten, Molybdenum, and Aluminum

From E - μ relation, we could see that for the isotropic material:

$$E = 2\mu(1 + \nu) \tag{27}$$

So, the ratio A could be regarded as a standard of anisotropic properties:

$$A = \frac{2\mu(1 + \nu)}{E} \tag{28}$$

The closer A is to 1, the more isotropic the material is. In our selections, the A of tungsten is 1.01, aluminum is 1.22, and molybdenum is 0.91.⁵

⁵The needed elasticity properties is derived from wikipedia.

4.2 Example: Computing the First Lamé Constant λ

The stress-strain relation for isotropic material is:

$$\sigma_{ij} = \lambda e_{kk} \delta_{ij} + 2\mu e_{ij}, \quad i, j = 1, 2, 3 \quad (29)$$

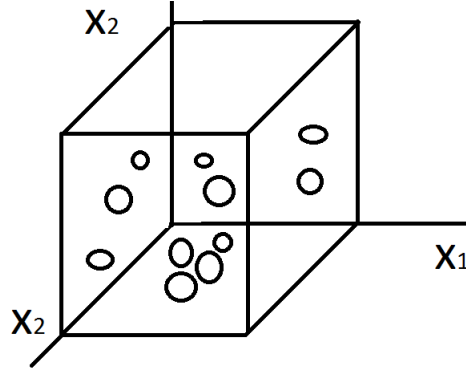


Figure 3: The scheme of deformation

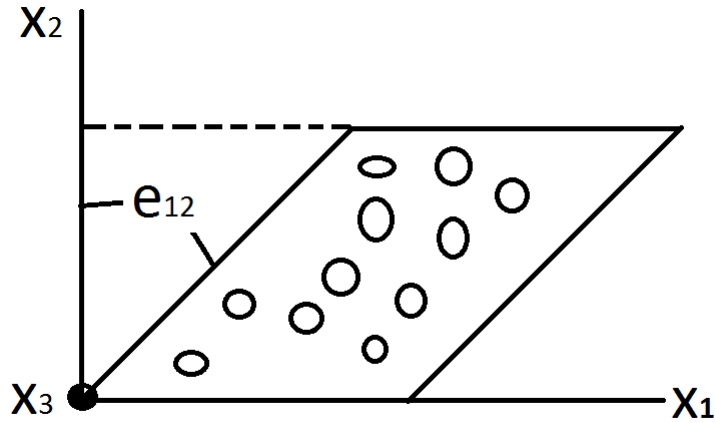


Figure 4: The scheme of deformation

When we apply the deformation in the simulation through x_1 , the strain in the x_1 direction could be directly obtained and the strain through x_2 and x_3 could also be derived if we set the conservation of mass condition.

Then:

$$\sigma_{11} = (\lambda + 2\mu)e_{11} + \lambda(e_{22} + e_{33}) \quad (30)$$

And for the shear case:

$$\sigma_{12} = 2\mu e_{12} \tag{31}$$

We obtain the stress through the derivative of internal energy and the strain due to our setting, and finally we could solve λ and μ as a system of linear equations.

4.3 The Use of Material Studio

The key point of our computation for the internal energy of material under deformation requires the software Material Studio. We have to do the simulation to obtain the thermodynamics properties using the Molecular Dynamics Module attached to the software. That's why we are applying the use of such software.