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Presentation of a Novel Method in the realm of Non-classical Continuum Mechanics Under the Vibration of Nano-scaled Structures

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Abstract

The following paper contains a presentation of a novel method to derive the lattice constitutive equation based on lattice basics. The lattice is assumed to be made of point masses and springs. In this method, a self-containing differential equation is presented, in which lattice parameter derivation, despite previous non-classical theories, is no longer difficult. The equation represents the displacement field of the lattice which is derived using the Taylor series. The order of the equation is determined by the number of terms in the Taylor series. Also, to compare the results, dispersion relation for a flexural beam in Eringen's non-local theory, Lattice model and the new method has been derived then the effect of lattice parameter- the distance between the point masses- on the dispersion curve has been investigated. Finally, the first three frequencies for the mentioned beam in these three methods in different boundary conditions have been derived and the error in each mode has been calculated.

Keywords: discrete dynamics; Lattice parameter; non-classical continuum; dispersion relation.

1. Introduction

Micro and nanostructures elements have a vast range of applications, especially as components in MEMS/NEMS. In all these applications, the atomic bond length of the micro and nanostructures is comparable to the dimensions of the structure. Due to the discrete structure of nanostructures, methods such as molecular dynamics are among the most accurate methods, but this method is computationally heavy and a costly process and time-consuming method for a high number of atoms. One can assume continuity to solve the system equation of motion, but when the wavelength of loading is comparable to the length of material, the size effect will become an important factor in the mechanical

modelling of the structures in which classical theories are unable to predict this phenomenon. Thus the size effect has an important role in deformation behavior of the structure and cannot be negligible.

As mentioned, classical continuum mechanics cannot predict the size effect in micro/nanostructures. To overcome this issue, some higher-order continuum theories which contain additional material length scale parameters besides the classical material constants, have been proposed to predict the size dependence of these structures. Most generally known higher-order theories are strain gradient elasticity [1], the non-local theory of Eringen [2], the micropolar (Cosserat) elasticity [3] and couple stress theories have been developed to characterize the size effect in micro/nanostructures by considering an intrinsic length scale in the constitutive relations.

In the theory of Micropolar elasticity by Cosserat brothers, additional rotational degrees of freedom at each material point in the body were considered. The classical couple stress theory is one of the other higher-order continuum theories which contains two additional material length scale parameters besides the classical constants for an isotropic elastic material, elaborated by Mindlin [4], Mindlin and Tiersten [5], Toupin [6], and Koiter [7]. In fact, couple stress theory is a particular case of Micropolar theory proposed by Cosserat brothers [3]. After the study was proposed by Koiter [7], some other researchers have made some development to this theory. Recently, a modified couple stress theory was proposed by Yang et al. [8] in which contains only one additional material length scale parameter in addition to the classical material constants.

The modified strain gradient elasticity theory is another higher-order continuum theory, which was proposed by Lam et al. [9] contains a new additional equilibrium equation besides the classical equilibrium equations and also five elastic constants (two classical and three non-classical) for isotropic linear elastic materials. Both the strain gradient elasticity and couple stress theories include the second-order displacement gradients.

Among these theories, the non-local elasticity theory, which was introduced by Eringen [10], has been widely used for modelling micro and nano-scaled structures to account for scale effect in elasticity. Finding the constants in mentioned theories has always been an issue for researchers; thus, in the field of non-classical continuum mechanics, this new method represents the governing equation on a structure which parameters have no difficulty in obtaining.

In the present paper, the behavior of a lattice as a basis of the subject has been explained then the presentation of the novel method according to the general 1D beam has been presented then the dispersion curves for each theory has been derived. Finally, the dispersion curve for different lattice parameters (wavelength) for the new method has been derived, and the results are discussed.

2. An overview of the vibration of nano-scaled solids

There are two types of methods for lattice analysis, (i) Discrete dynamics, (ii) Equivalent continuum model

In discrete dynamics, there are two types of methods in order to derive the differential equation of lattice, Newton, and Lagrange methods. In the Newton method, the equation of motion for a specific atom is acquired, then using the Bloch assumption ($u = \bar{U}e^{i(\kappa x+\omega t)}$), the governing differential equation on lattice will be derived. In the Lagrange method, the governing differential equation will be derived by obtaining the energy of the lattice. In discrete dynamics, applying boundary conditions are a challenge since one element is considered for it. If a limit length structure is considered, the equation of motion should be derived for every atom, which results in large matrixes.

Researchers have also presented various methods by assuming the structures as a continuum model. These methods rectify the continuum model to predict the behavior of a discrete model. Since, in the equivalent continuum method, a differential equation describes the behavior of the structure, researchers prefer to work on this area. In the following, these methods are presented.

2.1 Discrete Dynamics

An ideal crystal is constructed by the infinite repetition of identical groups of atoms Fig.1. A group is called the basis. The set of mathematical points to which the basis is attached is called the lattice. The lattice in three dimensions may be defined by three translation vectors a_1, a_2, a_3, such that the arrangement of atoms in the crystal looks the same when viewed from the point r as when viewed from every point r' translated by an integral multiple of the a's: [11]

$$r' = r + u_1 a_1 + u_2 a_2 + u_3 a_3 \quad \textbf{(1-2)}$$

Here u_1, u_2 and u_3 are arbitrary integers. The set of points r' for all u_1, u_2, u_3 defines the lattice.

The basis of the crystal structure can be recognized once the crystal axes have been chosen. Figure1 shows how a crystal is made by adding a basis to every lattice point; of course, the lattice points are just mathematical constructions. Every basis in a given crystal is identical to every other in composition, arrangement, and orientation. The number of particles within the basis may be one, or it may be more than one. The position of the center of a particle j of the basis relative to the associated lattice point is:

$$r_j = x_j a_1 + y_j a_2 + z_j a_3 \quad \textbf{(2-2)}$$

Thus, by taking a general lattice, as shown in the Figure1, the equation of motion for the reference atom can be derived as Eq. (3-2).

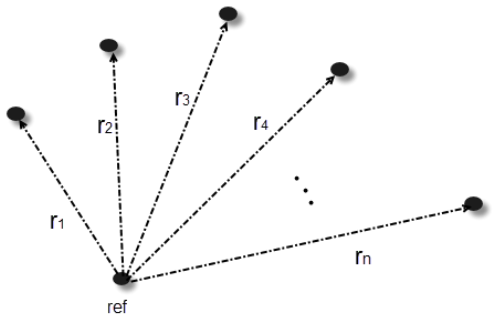

Figure 1. A Typical Lattice Schematic.

Thus the lattice constitutive equation can be written as below.

$$m\ddot{r_j} = \sum f_{ij} = \sum \frac{\partial}{\partial r_j} \phi(|r_i - r_j|) \quad \textbf{(3-2)}$$

Where ϕ is interatomic potential, and r_i is a function that specifies the location of each atom at time t.

Hamilton's principle is written for independent variations δu_i between fixed limits of u_i at times t_0 and t_1:

$$\delta \int_{t_0}^{t_1} (T - U)dt + \int_{t_0}^{t_1} \delta W dt = 0 \quad \textbf{(4-2)}$$

Where T and U are the total kinetic and potential energies in volume V and δW is the variation of work done by external forces.

The kinetic energy of the molecular lattice containing N atoms can be described as:

$$T = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{r}_i \,.\, \dot{r}_i \quad \textbf{(5-2)}$$

Where m_i is the mass of atom i.
Generally, the potential energy based on inter-atomic interactions can be separated into different terms depending on different atoms interactions as the following form:

$$E(r_1, r_2, \dots, r_m) = \sum_i \sum_{j>i} E_2(r_i, r_j) + \sum_i \sum_{j>i} \sum_{k>j>i} E_3(r_i, r_j, r_k) + \dots \quad \textbf{(6-2)}$$

Where r_i stands for the position of atom i, and E_2 and E_3 are two and three atoms interactions potentials. Assuming that three and more atoms interactions potentials are negligible, the potential energy will become as follow:

$$E(r_1, r_2, \dots, r_m) = \sum_i \sum_{j>i} E_2(r_i, r_j) \quad \textbf{(7-2)}$$

Then by substituting interatomic forces with tensional and torsional springs, the total potential will be as:

$$U = \frac{1}{2} \sum_{i=1}^{N} \sum_{j>i}^{N} K_{ij}(r_i - r_j)^2 + \frac{1}{2} \sum_{i=1}^{N} \sum_{j>i}^{N} K_\theta(\theta_i - \theta_j)^2 \quad \textbf{(8-2)}$$

Where K_{ij} is equivalent stiffness between atoms i and j.
For longitudinal vibration analysis of lattice we obtain:

$$T = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{r}_i . \dot{r}_i \quad \textbf{(9-2)}$$

$$U = \frac{1}{2} \sum_{i=1}^{N} K_{\delta i}((r_{i+1} - r_i)^2 + (r_{i-1} - r_i)^2) \quad \textbf{(10-2)}$$

For lateral vibration analysis of lattice we obtain:

$$T = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{\theta}_i . \dot{\theta}_i \quad \textbf{(11-2)}$$

$$U = \frac{1}{2\delta} \sum_{i=1}^{N} K_{\theta i}(\theta_{i+1} + \theta_{i-1} - 2\theta_i)^2 \quad \textbf{(12-2)}$$

Therefore, the governing equations of motion are obtained using the Hamilton principal:

$$m\ddot{u}_n - k_\delta(u_{n+1} + u_{n-1} - 2u_n) = 0 \quad \textbf{(13-2)}$$

$$m\ddot{w}_n + \frac{k_\theta}{\delta^2}(\theta_{n+2} + 4\theta_{n+1} + 6\theta_n - 4\theta_{n-1} + \theta_{n-2}) = 0 \quad \textbf{(14-2)}$$

3. Presentation of a new method

In a 3D solid, imagine that $x_i + y_j + z_k$ represents the position of an atom. Imagine that the vector field (u_i, v_j, w_k, t) is a continuum field which interpolates the position of each particle.

To relate continuum theories of elasticity to general atomic or molecular theories, one needs some way of relating changes in positions of the entities.

This novel method, which is based on equivalent lattice stiffness, represents a self-containing differential equation that finds its parameters due to the lattice parameter, based on continuum mechanics and lattice dynamics concepts. For this purpose, a lemma should be considered:

Lemma: Continuum model is a hypothesis that surrounds the particles used in the mathematical formulation of solid mechanics, which relates the movement of atoms in a crystal to the overall deformation of the bulk solid.

This method presents a continuous function that surrounds particles and interpolates the movement of atoms in a crystal.

$$r_i = r_0 + e(x, y, z, t)|_{r0} \tag{1-3}$$

In which e is a continuous function that interpolates the movement of the particles, and r_i is the position of an atom and can defined as:

$$r_i = x_i + y_j + z_k \tag{2-3}$$

3.1 Governing Equations

In order to obtain the position of an atom, one should derive the governing differential equation of the particle.

$$[M]\begin{Bmatrix}\ddot{u}\\ \ddot{v}\\ \ddot{w}\end{Bmatrix} + [K]\begin{Bmatrix}u\\ v\\ w\end{Bmatrix} = \vec{F} \tag{3-3}$$

Then extending the equation by substituting tailor expansion and assuming smooth waves, it results in a differential equation of order n which has the form like equation below:

$$[M]\begin{Bmatrix}\ddot{u}\\ \ddot{v}\\ \ddot{w}\end{Bmatrix} + [D]\begin{Bmatrix}u\\ v\\ w\end{Bmatrix} = \vec{F} \tag{4-3}$$

In which D is a differential operator that forms the lattice parameters automatically.

One of the most widely used structures are nano-beams. In the following the schematic of a 2D chain which can carry tensile and bending loadings can be seen in Fig.2.

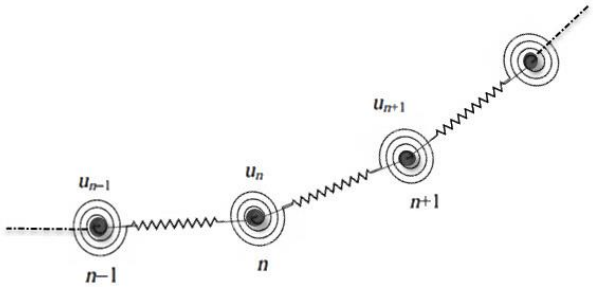

Figure 2. A Typical 2D Beam Schematic.

The equations of motion for a general 2D lattice (chain) assuming two types of interatomic potential including bond stretch and torsional potentials, can be described as:

$$\begin{cases} m(x)u_{,tt} - (EA(x)u_{,x})_{,x} = 0 \\ m(x)w_{,tt} + EI(x)w_{,xxxx} = 0 \end{cases} \tag{5-3}$$

Axial, bending stiffness and mass per length are defined as:

$$\begin{cases} k_\delta = \dfrac{EA}{\delta} \\ k_\theta = \dfrac{EI}{\delta} \\ m = \rho A \delta \end{cases} \tag{6-3}$$

Assuming constant section along with the structure, the equations will be transformed to:

$$\begin{cases} \rho A u_{,tt} - k_\delta u_{,xx} = 0 \\ \rho A w_{,tt} + k_\theta w_{,xxxx} = 0 \end{cases} \quad \textbf{(7-3)}$$

Then extending the equation by substituting Taylor series and assuming smooth waves, it results in a differential equation of order n which has the form like equation below:

$$m\ddot{u}_n - k_\delta \left(\delta^2 u''_n + \frac{\delta^4}{12} u^{(4)}{}_n + 2 \sum_{i=3}^{\infty} \frac{\delta^{2i}}{(2i)!} u_n{}^{(2i)} \right) = 0 \quad \textbf{(8-3)}$$

$$m\mathrm{w}_n - k_\theta \left(\delta^2 w^{(4)}{}_n + \frac{\delta^4}{6} w^{(6)}{}_n + \frac{\delta^6}{80} w^{(8)}{}_n + \cdots \right) = 0 \quad \textbf{(9-3)}$$

4. Numerical Investigation

Any existent microstructural heterogeneity of crystalline materials affects the dispersion of elastic waves, which is a real physical phenomenon that can be observed and studied experimentally. The shape of a general propagating wave changes over time due to the different propagating speeds of different harmonic components in it. This phenomenon is commonly known as dispersion. The dispersion relation is the relationship between the frequency of vibrations and the wave-vector κ. The dispersion relation is not related to the boundary conditions; thus, this is one of the methods to obtain bulk material properties.

In the following, the dispersion curves for a flexural beam has been obtained. The dispersion relation for a flexural lattice beam is as below:

$$\frac{\omega}{\Omega} = \sqrt{16\sin^2 \frac{\kappa\delta}{2} - 4sin^2\kappa\delta} \quad \textbf{(1-4)}$$

The dispersion relation for the mentioned beam in non-local theory is as below:

$$\frac{w}{\Omega} = (\kappa\delta)^2 (1 + {e_0}^2 \kappa^2 \delta^2)^{-\frac{1}{2}} \quad \textbf{(2-4)}$$

The matching is perfect at $e_0 = 0.39$. [10] Then by comparing these equations, we get:

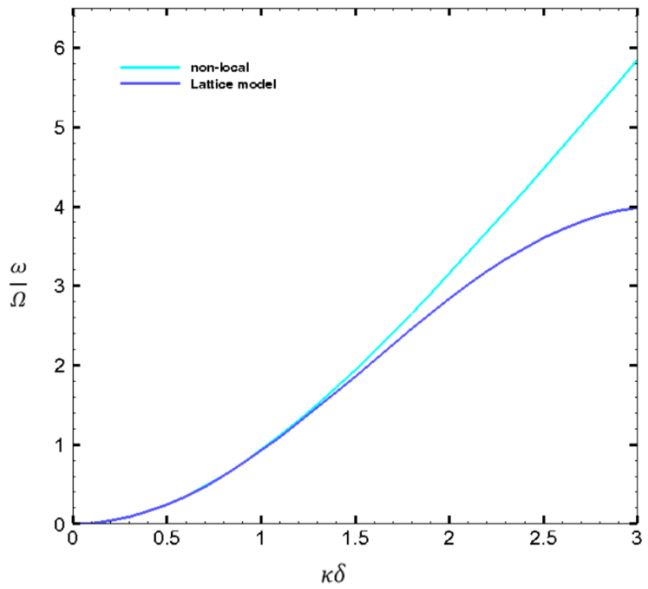

Figure 3. Dispersion curve comparison for non-local and Lattice model in a flexural beam

In the following, the dispersion relation of the beam is presented by the new method:

$$\frac{\omega}{\Omega} = \kappa^2\delta^2\sqrt{1-\frac{\kappa^2\delta^2}{6}} \qquad \textbf{(3-4)}$$

Then by comparing this equation to those of Fig.6, we get.

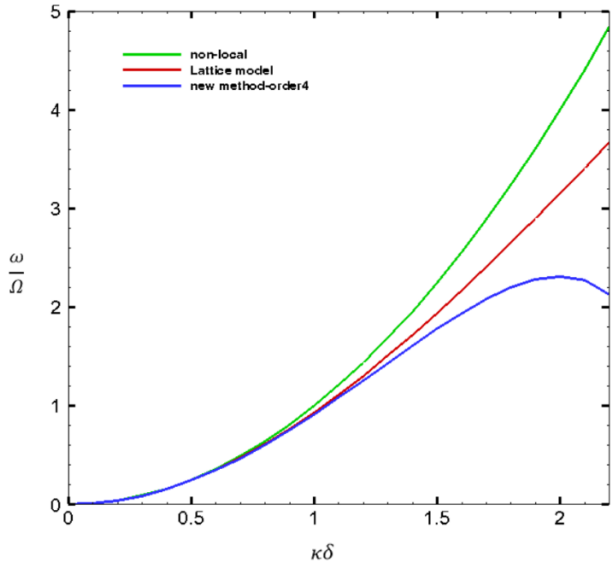

Figure 4. Dispersion curve comparison for non-local, Lattice model and the presented method in a flexural beam

In the following, the dispersion curves for various orders of the new method have been plotted.

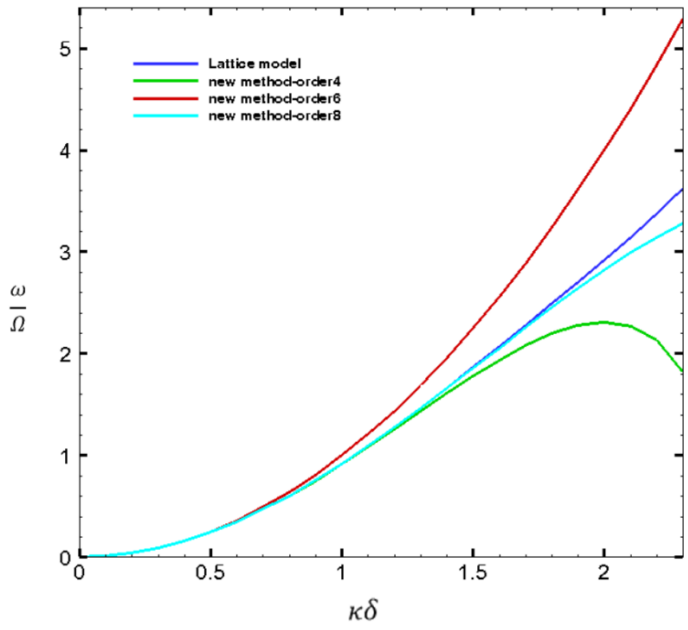

Figure 5. Dispersion curve comparison for Lattice model and the presented method in a flexural beam

As can be seen, the more the order goes in this method, the curves become closer to the lattice curve, which in order8, it almost becomes fitted to the lattice curve.

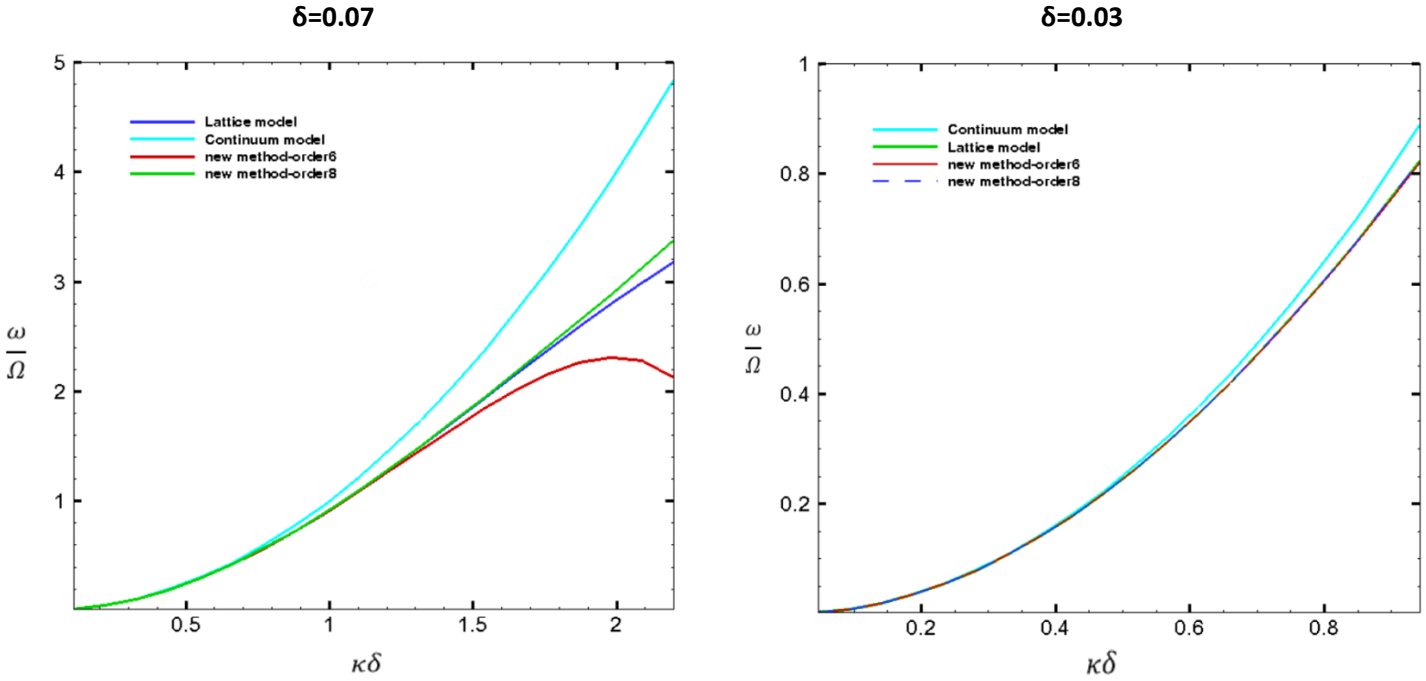

Figure 6. Comparison between the dispersion curves of a flexural beam with δ=0.03 and δ=0.07

As can be seen by decreasing the lattice parameter, the curves obtained from the new method become closer to the continuum model.

In the following, the value of frequencies of different modes in different conditions for the finite element model of a beam and different orders of the presented method have been compared. Thus, the frequencies for the first three modes of a lattice have been compared to those obtained from the presented method of order 4 and 6.

Table 1. Frequency comparison of Lattice model and the presented method in a beam with C-C B.C.

Mode	Lattice Frequency(Hz)	New method-Order4 Frequency(Hz)		New method-Order6 Frequency(Hz)	
		value	Error%	Value	Error%
1	22.82	22.371	0.01	22.373	0.01
2	62.91	61.64	0.02	61.67	0.01
3	123.30	120.8	0.02	120.9	0.01

Furthermore, the frequencies for the first three modes of a lattice have been compared to those obtained from the new method of order 4 and 6.

Table 2. Frequency comparison of Lattice model and the presented method in a beam with C-S B.C.

Mode	Lattice Frequency(Hz)	New method-Order4 Frequency(Hz)		New method-Order6 Frequency(Hz)	
		value	Error%	Value	Error%
1	15.57	15.41	0.01	15.4167	0.009
2	50.92	49.94	0.02	49.96	0.01
3	106.09	104.166	0.02	104.248	0.01

5. Conclusion

The features of the presented paper are as follow:

- Presentation of a novel method to derive the general lattice constitutive equation based on Taylor series which results in a self-containing differential equation
- Derivation of a differential equation of a general beam using the novel method
- Studying the dispersion curves of different orders of the presented method and non-local theory and obtaining the experimental constant
- Studying the frequency of C-C and C-S beam versus lattice parameter for the first three modes
- Studying the effect of lattice parameter on the accuracy of dispersion curves approximation

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