
# MECHANICAL BEHAVIOR OF ATOMS USING ATOMIC-SCALE FINITE ELEMENT METHOD

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**Abstract.** *This paper revisits the Atomic-scale Finite Element Method (AFEM) formulated in the article by Liu et al., (2004) which describes the mechanical behavior of a set of atoms. We proposes a new arrangement for the elements, for the inclusion of the boundary conditions and also exploits the idea of linking the size of the atomic-scale element to the concept of cut-off radius applied in Molecular Dynamics (MD) simulations. The AFEM is formulated based on the concept of potentials describing the interaction among atoms. Opposite to traditional local character of the element concept within the frame of FEM, the potentials used to generate the AFEM have non-local character. The article presents a formulation for 1D and 2D atomic-scale elements in which this non-local character of the potential interaction between atoms is considered. In the present implementation the Lennard-Jones pair potential is used to calculate the total energy of the system. AFEM uses both first and second derivatives from a molecular force field to derive, respectively, the load vector and system stiffness matrix. The resulting non-linear system is solved iteratively. Force-strain relations are obtained numerically. The numerical results obtained from the procedure proposed in this work are compared to a standard MD implementation based on the LAMMPS software. Accuracy, convergence and numbers of iterations of the AFEM compared to MD are addressed. The proposed methodology can be extended to more complex interatomic potentials, for instance REBO or ReaxFF, which can describe the mechanical behavior of nano-carbon structures such as nano-whiskers and nano-tubes.*

***Keywords:*** *Atomic-scale finite element method, Molecular Dynamics, Lennard-Jones Potential*

# 1 INTRODUCTION

According to the definition given by the Royal Society and the Royal Academy of Engineering (2004), "nanotechnologies are the design, characterization, production and application of materials, structures, devices and systems by controlling their shape and size at the nanometer scale. Nanomaterials are categorized as those that have structured components with at least one dimension in the 1-100 nm range". Nanotechnology has made many advances in materials, electronics, biology and medicine. According to Dewapriya (2012) "recently, researchers were able to manipulate a single atom in a way they want, which will lead researchers to fabricate devices by manipulating atom by atom. Isolation of a single layer graphene sheet from bulk graphite started a new research front in nanotechnology".

The conventional continuum methods such as the finite element method (FEM) are not applicable to nanoscale components. The key idea of this article is to revisit a formulation of the atomic-scale finite element method (AFEM), proposed by Liu et al., (2004), for one and two dimensional analysis of the mechanical behavior of set of atoms using the Lennard-Jones pair potential, which describes the interaction between two atoms within a distance called the cut-off radius. Distinct AFEM elements for 1 and 2 dimensions are developed based on the cut-off radius concept, present in the in Lennard-Jones potential, and the atomic lattice. Numerical results for force – strain relation, relative and absolute error are compared to a standard Molecular Dynamics implementation based on the LAMMPS software (Plimpton et al., 2007). Convergence and iteration's number are also analysed.

# 2 LENNARD JONES POTENTIAL

In this section, a brief review of the Lennard-Jones potential is introduced. The AFEM formulation implemented in this article is based on this pair-wise potential. The Lennard-Jones potential, proposed by Sir John Edward Lennard-Jones (Jones, 1924), describes the potential energy of interaction between two non-bonding atoms based on their distance of separation. It is particularly accurate for noble gases. Lennard Jones potential is given by:

$$U\left(r\right) = 4\,\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1}$$

In this potential, the parameter $\varepsilon$ is the depth of the potential well and $\sigma$ is the inter-particle distance at which the potential is zero. The distance between the two considered atoms is denoted by $r$. The Lennard-Jones model consists of two terms: the $(\sigma/r)^{12}$ term, which is the repulsive term and the $(\sigma/r)^{6}$ term, which is the attractive term, and two independent parameters: $\sigma$ with the dimension of length (Å = $10^{-10}$ m) and $\varepsilon$ with the dimension of energy ( eV = $1.60217733 \cdot 10^{-19}$ J) . The intermolecular force between the two atoms $F(r)$ is obtained by differentiating the potential with respect to the intermolecular distance, $r$:

$$F\ (r) = -\ \frac{\partial\ U(r)}{\partial\ r} = 4\ \varepsilon\ \left[12\ \frac{\sigma^{12}}{r^{13}}\ -\ 6\ \frac{\sigma^{6}}{r^{7}}\right] \tag{2}$$

As will be detailed later in this article, the second derivative of the interatomic potential corresponds to a stiffness-like matrix. For the L-J potential, the second derivative is:

$$K\ (r)\ =\ \frac{\partial^2\ U\ (r)}{\partial\ r^2} = 4\ \varepsilon\ \left[156\ \frac{\sigma^{12}}{r^{14}}\ -\ 42\ \frac{\sigma^{6}}{r^{8}}\right] \tag{3}$$

Figure 1 shows the variation of L-J potential $U(r)$ and the interatomic force $F(r)$ with the distance, *r*. By setting the force $F(r) = 0$, the equilibrium distance between the atoms, $r_{eq}$ is found to be:

$$r_{eq}\ =\ 2^{\frac{1}{6}}\ \sigma\ =\ 1.1225\ \sigma \tag{4}$$

If the distance between two atoms is less than $r_{eq}$, the Lennard-Jones force is repulsive. If the distance is greater than $r_{eq}$, the force is attractive. The maximal force is obtained at the intermolecular distance

$$r_{f\,\max}\ =\ \frac{1}{\sqrt[6]{\frac{7}{26}}}\ \sigma\ =\ 1.2445\ \sigma \tag{5}$$

An important feature of the molecular dynamics simulation using the L-J potential is the concept of a cut-off radius, $r_c$. It is a chosen parameter and represents the distance an atom influences and is influenced by others. Conceptually, the L-J potential U defined in Eq. (1) is considered to be zero if $r \geq r_c$. This idea, which will be connected to the number of nodes of the proposed atomistic finite element (AFEM) is illustrated in the Fig. 2a to 2d.

Consider Fig. 2a, which shows a 1D atomic chain with 5 equal atoms in equilibrium. The equilibrium distance between the neighboring atoms is denoted by $r_{eq}$. Assume now that this problem will be addressed by the L-J potential assuming a cut-off radius $r_c$ satisfying the condition ($r_{eq} < r_c < 2r_{eq}$). This means that one atom only interacts with its closest neighboring atoms. This is pictorially shown in Fig. 2b. Now consider the same atomic chain is modelled with a cut-off radius ($2r_{eq} < r_c < 3r_{eq}$). Under this circumstance, every atom interacts with its 2 neighboring atoms on each side, as depicted in Fig. 2c. An analogous situation, showing the interatomic interaction for the condition ($3r_{eq} < r_c < 4r_{eq}$) is shown in Fig. 2d.

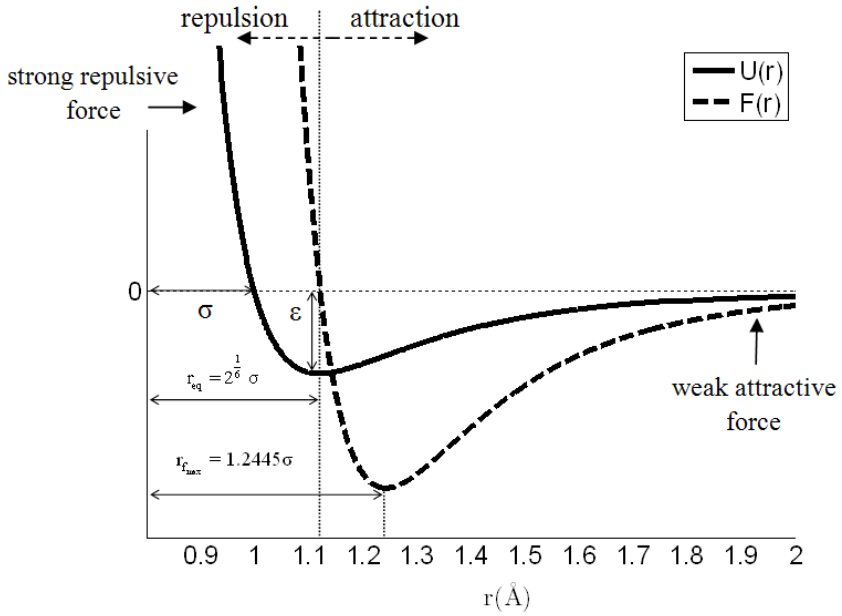


**Figure 1: Lennard-Jones inter-atomic potential U(r) and resulting force field F(r).**

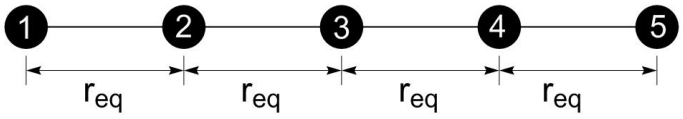


**Figure 2a: A chain with 5 atoms in equilibrium at the intermolecular distance $r_{eq}$ .**

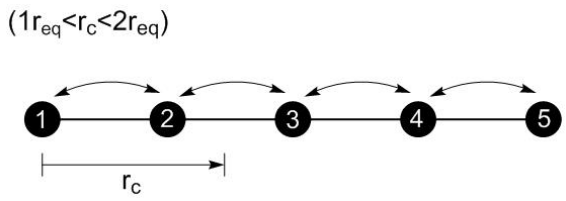


**Figure 2b: For the condition ($1r_{eq} < r_c < 2r_{eq}$) one atom interact only with the closest neighboring atoms**

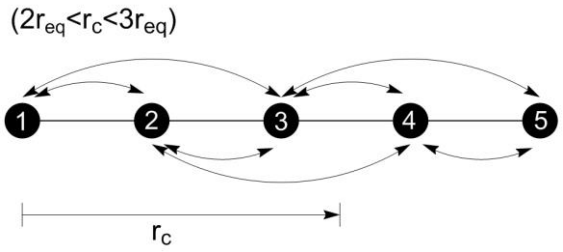


**Figure 2c: For the condition ($2r_{eq} < r_c < 3r_{eq}$) one atom interact with the two closest neighboring atoms**

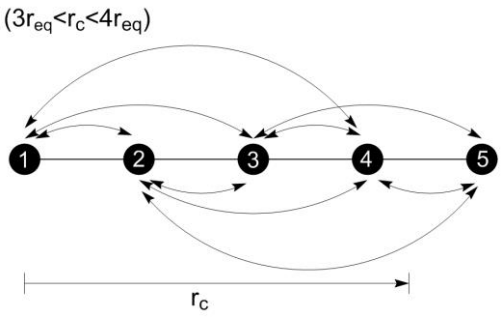


**Figure 2d: For the condition ($3r_{eq} < r_c < 4r_{eq}$) one atom interact with the three closest neighboring atoms**

# 3 THE ATOMIC-SCALE FINITE ELEMENT METHOD (AFEM)

AFEM, as proposed by Liu et al., (2004), is formulated by finding a state of minimum total energy $E_{tot}$ of the system under analysis with respect to the vector describing the position of the atoms, $\underline{x}$.

$$\frac{d\, E_{tot}}{d\, \underline{x}} = 0 \tag{6}$$

The total system energy is comprised of the internal energy stored within the atomic bonds, $U$, and the work done by the external forces, $W_f$. For a system with $N$ atoms the internal interatomic energy is given by:

$$U_{tot} = \sum_{i<j}^{N} U\left(\underline{x}_j - \underline{x}_i\right) \tag{7}$$

In equation (7) $U$ denotes an interatomic potential such as the described Lennard-Jones. Considering the external force $\underline{F}_i$ acting on the $i^{th}$ atom, the work done by the external forces may be written as:

$$W_f = \sum_{i=1}^{N} \underline{F}_i \bullet \underline{x}_i \tag{8}$$

Considering equation (7) and (8) the total energy of the system is given by:

$$E_{tot} = \sum_{i<j}^{N} U\left(\underline{x}_j - \underline{x}_i\right) - \sum_{i=1}^{N} \underline{F}_i \bullet \underline{x}_i \tag{9}$$

The total energy $E_{tot}$ can be expanded in a Taylor series around the equilibrium point $\underline{x}^{(0)}$:

$$E_{tot}\left(\underline{x}\right) \approx E_{tot}\left(\underline{x}^{(0)}\right) + \left.\frac{d\, E_{tot}}{d\, \underline{x}}\right|_{\underline{x}\,=\,\underline{x}^{(0)}} \left(\underline{x}-\underline{x}^{(0)}\right) + \frac{1}{2}\left(\underline{x}-\underline{x}^{(0)}\right)^T \left.\frac{d^2 E_{tot}}{d\, x\, d\, x}\right|_{\underline{x}\,=\,\underline{x}^{(0)}} \left(\underline{x}-\underline{x}^{(0)}\right) \tag{10}$$

Defining the displacement $\underline{u}$ as:

$$\underline{u} = \left(\underline{x} - \underline{x}^{(0)}\right) \tag{11}$$

Expression (10) can be expressed as:

$$E_{tot}\left(\underline{x}\right) \approx E_{tot}\left(\underline{x}^{(0)}\right) + \left.\frac{\partial E_{tot}}{\partial \underline{x}}\right|_{x=x^{(0)}} \underline{u} + \frac{1}{2}\,\underline{u}^{T}\left.\frac{\partial^2 E_{tot}}{\partial \underline{x}\,\partial \underline{x}}\right|_{x=x^{(0)}} \underline{u} \tag{12}$$

Looking for a stationary value of the total energy given in equation (12), it is possible to write:

$$\frac{\partial E_{tot}}{\partial \underline{x}} = \frac{\partial E_{tot}}{\partial \underline{u}} \approx \frac{\partial}{\partial \underline{u}}\left[E_{tot}\left(\underline{x}^{(0)}\right) + \left.\frac{\partial E_{tot}}{\partial \underline{x}}\right|_{x=x^{(0)}} \underline{u} + \frac{1}{2}\,\underline{u}^{T}\left.\frac{\partial^2 E_{tot}}{\partial \underline{x}\,\partial \underline{x}}\right|_{x=x^{(0)}} \underline{u}\right] \tag{13}$$

This expression can be evaluated to yield:

$$\frac{\partial E_{tot}}{\partial \underline{x}} \approx \frac{\partial E_{tot}}{\partial \underline{x}}\left(\underline{x}^{(0)}\right) + \left.\frac{\partial^2 E_{tot}}{\partial \underline{x}\,\partial \underline{x}}\right|_{x=x^{(0)}} \underline{u} = 0 \tag{14}$$

Substituting (9) into (14) results in:

$$\left.\frac{\partial U_{tot}}{\partial \underline{x}}\right|_{\underline{x}=\underline{x}^{(0)}} - \underline{F}_i + \left.\frac{\partial^2 U_{tot}}{\partial \underline{x}\,\partial \underline{x}}\right|_{\underline{x}=\underline{x}^{(0)}} \underline{u} = 0 \tag{15}$$

This expression can be written as:

$$\underline{K}\left(\underline{u}\right)\,\underline{u} = \underline{P} \tag{16}$$

with the stiffness matrix $\underline{K}\,(\underline{u})$ and the non-equilibrium load vector $\underline{P}$, respectively given by:

$$\underline{K}\left(\underline{u}\right) = \left.\frac{d^2 U_{tot}}{d\,\underline{x}\,d\,\underline{x}}\right|_{\underline{x}=\underline{x}^{(0)}} \tag{17}$$

$$\underline{P} = \underline{F}_i - \left.\frac{d\,U_{tot}}{d\,\underline{x}}\right|_{\underline{x}=\underline{x}^{(0)}} \tag{18}$$

This is the basic formulation for the AFEM, based on interatomic potentials. In general the system described by equation (16) is non-linear and must be solved iteratively (Owen and Hinton, 1980). In the next session the idea of an atomic-scale element is addressed.

# 4 ATOMIC-SCALE FINITE ELEMENTS

**1D case**.The element notion that is proposed in this work starts with the idea that pair-wise potentials are being used, which describes the internal energy between two interacting atoms. Atomic-scale elements are defined by a central node (atom) a surrounding nodes (atoms) which are influenced by the central atom. The number of atoms that are influenced by the central atom (node) depends on the assumed cut-off radius of the interatomic potential. This is illustrated in Figures 2a through 2c, for one dimensional element. Consider Fig. 3a. This is a 3-node atomic finite element. The central node (atom) is designated by (*i*) and its surrounding atoms (nodes) are (*i-1*) and (*i+1*). It should be clear that this element corresponds to the use of a cut-off radius, $r_c$, expressed by the condition ($r_{eq} < r_c < 2r_{eq}$), as shown in Fig. 3a. The arrows shown in Fig. 3a for this element indicate that the bonding energy to be considered is that describing the influence of element (*i*) on the neighboring (*i-1*) and (*i+1*). The influence of atom (*i-1*) on the atom (i) and the element of atom (*i+1*) on (*i*) is considered at a later stage, at the assembly of the atomic elements. So only half of the bonding energy between (*i*) and (*i-1*) has to be considered. Analogously only half of the bonding energy between (*i*) and (*i+1*) is taken into account. This will be considered by the 1/2 factor in the element stiffness matrix.

The total potential energy of the 3-node element is given by:

$$U_{tot}^{i} = U_{i,i-1} + U_{i,i+1} \tag{19}$$

Expression (19) may be used in conjunction with equation (17) to build the stiffness matrix and the load vector for the 3-node element. The expressions for the 3x3 stiffness matrix $K^{3e}$ and the 3x1 load vector $P^{3e}$ are, respectively:

$$\underline{K}_i^{3e} = \begin{bmatrix} 0 & \frac{1}{2}\frac{d^2 U_{tot}}{d x_{i-1} d x_i} & 0 \\ \frac{1}{2}\frac{d^2 U_{tot}}{d x_{i-1} d x_i} & \frac{d^2 U_{tot}}{d x_i d x_i} & \frac{1}{2}\frac{d^2 U_{tot}}{d x_{i+1} d x_i} \\ 0 & \frac{1}{2}\frac{d^2 U_{tot}}{d x_{i+1} d x_i} & 0 \end{bmatrix}_{3x3} \tag{20}$$

$$\underline{P}_i^{3e} = \begin{bmatrix} 0 \\ \overline{F} - \dfrac{d\,U_{tot}}{d\,x_i} \\ 0 \end{bmatrix}_{3x1} \tag{21}$$

Atomic-scale elements with 5 and 7 nodes (atoms) can be built and are pictorially shown in Figures 3b and 3c. These elements represent the interatomic bonds in which the potential cut-off radius is, respectively, ($2r_{eq} < r_c < 3r_{eq}$) and ($3r_{eq} < r_c < 4r_{eq}$). The total bonding potential energy of the elements with 5 and 7 nodes are, respectively (see Figures 3b and 3c):

$$U_{tot}^{i-5e} = U_{i,i-1} + U_{i,i-2} + U_{i,i+1} + U_{i,i+2} \tag{22}$$

$$U_{tot}^{i-7e} = U_{i,i-1} + U_{i,i-2} + U_{i,i-3} + U_{i,i+1} + U_{i,i+2} + U_{i,i+3} \tag{23}$$

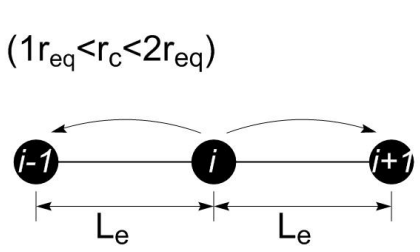


**Figure 3a: A three-node atomic-scale finite element used for the condition (req< rc <2req)**

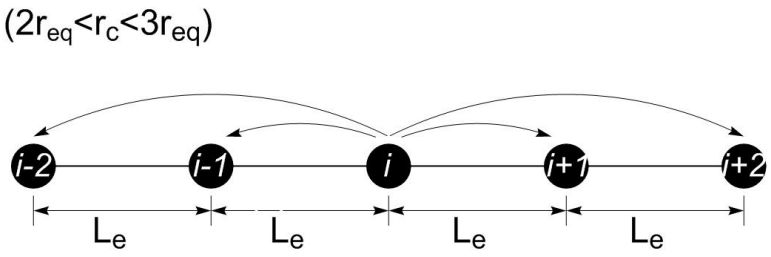


**Figure 3b: A five-node atomic-scale finite element used for the condition (2req< rc <3req)**

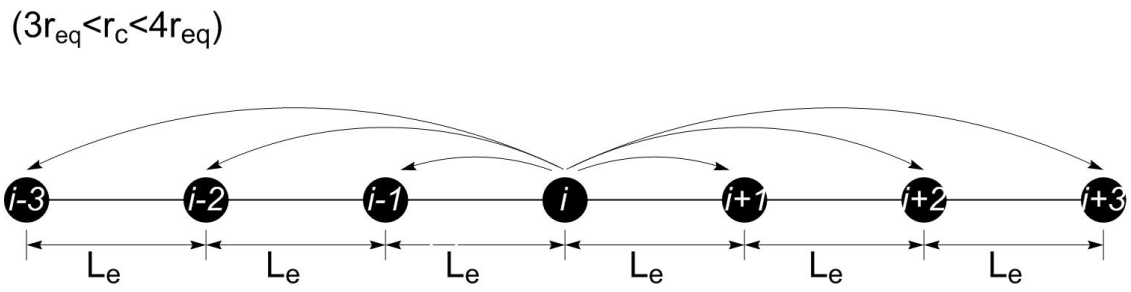


**Figure 3c: A seven-node atomic-scale finite element used for the condition (3req< rc <4req)**

**The stiffness matrix assembly procedure.** Figure 4 illustrates the AFEM assemblage procedure for an atomic chain containing 4 atoms. In this example the cut-off radius of the inter-atomic potential obeys the relation ($r_{eq} < r_c < 2r_{eq}$). For this case, 4 elements (*El*) with 3 nodes are used. The element stiffness matrices ($K_i^{3e}$) is superposed exactly as in the classical FEM. The top drawing in figure 4, shows the atomic chain with 4 atoms and the arrows show the inter-atomic interaction. In this case atom 1 influences atom 2 and vice-versa. The

superposition of the stiffness matrices of element 1 (*El* = 1) and element 2 (*El* = 2) will fully describe this reciprocal bond.

An important issue in the assemblage procedure is related to the atoms at the extremities of the atomic chain. In the present example, atoms 1 and 4. There is no atom to the left of atom 1. So the contribution of the central node (0) of the first atomic element (*El* = 1) onto its left node (-1) does not exist and this contribution must be excluded from the element stiffness matrix ($K_1^{3e}$). This is indicated by the dashed arrow linking nodes (0) and (-1) of the first element (*El* = 1). Analogously, the contribution from the central node (0) to the right node (+1) of the 4th element ($K_4^{3e}$) must be excluded from the assemblage procedure. This is also indicated in the last drawing of Fig. 4. This is an important issue in assembling the AFEM. The influence (bonding energy) of the nodes for the elements at the extremities of the atomic chain must excluded from the assemblage procedure. From the programming point of view, this operation resembles the inclusion of prescribed zero-displacement boundary conditions (zero Dirichlet boundary conditions) in the classical FEM.

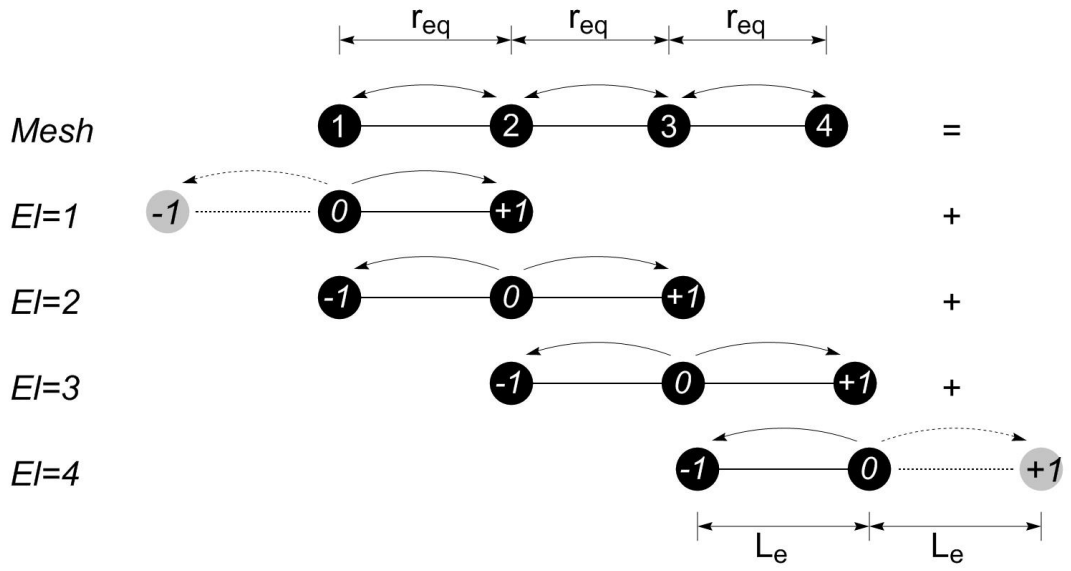


**Figure 4: Example of assemblage scheme for 4 atoms using 4 atomic elements with 3 nodes, used under the condition that ($1r_{eq}<r_{ec}<2r_{eq}$). Note the AFEM nodes that will not be taken into account at the assembly process. (Element 1, node -1, Element=4, node=+1)**

**Boundary Conditions for the AFEM**. The procedure described in the preceding paragraphs, which explains how to treat the contributions of the atoms of the extremities of the chain to the assembly procedure, should not be confused with the introduction of the displacement (Dirichlet) or force (Newman) boundary conditions on the atomic chain. Fig. 5 shows the boundary conditions imposed on the same atomic chain of figure 4. Now the displacement of the first atom (1) is blocked and its contribution must also be excluded from the global stiffness matrix, as in the classical FEM. From the programming point of view, these two operations (excluding influence of non-physical nodes at extreme elements and the imposition of zero-displacement boundary conditions at some atoms at the extremity) are very similar. But conceptually they are completely distinct.

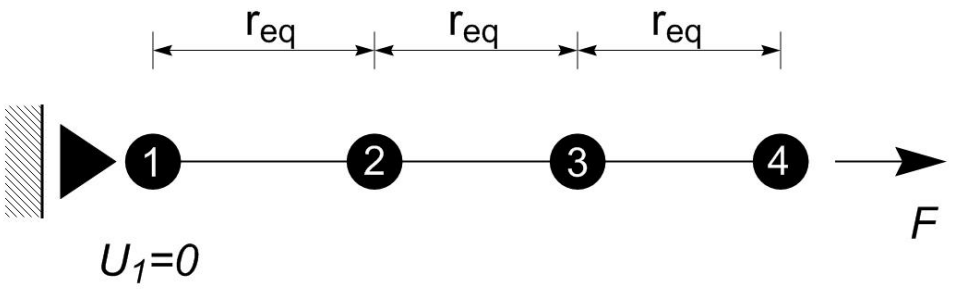


**Figure 5: Introduction the boundary conditions at the 4 atoms chain.**

**The 2D case**. It is possible to extend the atomic-scale finite element that was formulated in the preceding paragraphs to the two-dimensional and even to the 3D case. In this session we describe the 2D AFEM for a pair-wise potential interaction, like Lennard-Jones potential. Figure 6 shows the 2D AFEM for the case in which the potential cut-off radius obeys the restriction ($r_{eq} < r_c < 2r_{eq}$). It a natural extension of the 1D element shown in Fig. 3a. The element has one central node ($i$) and 6 surrounding nodes ($i+1$) to ($i+6$). The bonds to be considered in this element are between the central atom ($i$) and all its neighbors. There are no bonds between any of the nodes surrounding the central node. For instance, there is no bonding between node (i+1) and (i+2). The total element potential energy, the stiffness matrix and the loading vector for this element are given by:

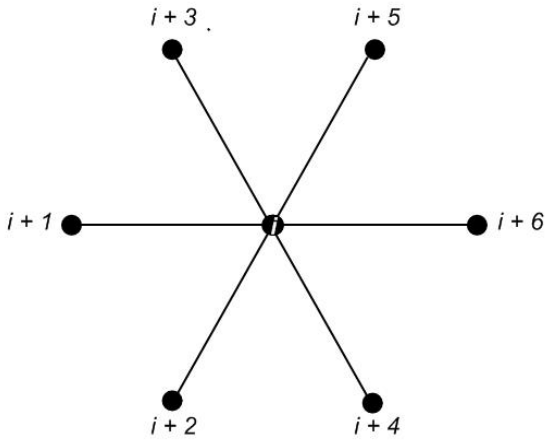


**Figure 6: A 2D AFEM with 7 nodes for ($1r_{eq} < r_c < 2r_{eq}$)**

$$U_{tot}^{2D-7} = U_{12} + U_{13} + U_{14} + U_{15} + U_{16} + U_{17} \tag{24}$$

and

$$\underline{K}_i^{2D-7} = \begin{bmatrix} 0 & \cdots & 0 & \frac{d^2 U_{tot}}{d x_1 d x_4} & \frac{d^2 U_{tot}}{d x_1 d y_4} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \frac{d^2 U_{tot}}{d y_1 dx_4} & \frac{d^2 U_{tot}}{d y_1 d y_4} & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \vdots & \vdots & 0 & \cdots & 0 \\ \frac{d^2 U_{tot}}{d x_1 d x_4} & \frac{d^2 U_{tot}}{d x_1 d y_4} & \cdots & \frac{d^2 U_{tot}}{d x_4 d x_4} & \frac{d^2 U_{tot}}{d y_4 d x_4} & \cdots & \frac{d^2 U_{tot}}{d x_7 d x_4} & \frac{d^2 U_{tot}}{d y_7 d x_4} \\ \frac{d^2 U_{tot}}{d y_1 dx_4} & \frac{d^2 U_{tot}}{d y_1 d y_4} & \cdots & \frac{d^2 U_{tot}}{d x_4 d y_4} & \frac{d^2 U_{tot}}{d y_4 d y_4} & \cdots & \frac{d^2 U_{tot}}{d x_7 d y_4} & \frac{d^2 U_{tot}}{d y_7 d y_4} \\ 0 & \cdots & 0 & \vdots & \vdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \frac{d^2 U_{tot}}{d x_7 d x_4} & \frac{d^2 U_{tot}}{d x_7 d y_4} & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \frac{d^2 U_{tot}}{d y_7 dx_4} & \frac{d^2 U_{tot}}{d y_7 d y_4} & 0 & \cdots & 0 \end{bmatrix}_{14x14} \tag{25}$$

$$\underline{P}_i^{2D-7} = \begin{bmatrix} (0)_{6x1} \\ \overline{F} - \frac{d U_{tot}}{d x_4} \\ \overline{F} - \frac{d U_{tot}}{d y_4} \\ (0)_{6x1} \end{bmatrix}_{14x1} \tag{26}$$

Assemblage of the 7-node 2D element. The drawings in Fig. 7 show the assemblage process for a chain of atoms of the same form of the original 7-node 2D element. In this drawings, the element central node is indicated by a full black filling. The neighboring nodes are filled with gray. Seven elements must be superposed to build a chain with the same arrangement of the considered element. The last drawing indicates the physical mesh with 7 atoms that is built with 7 elements. The central node of the element is place on every node of the mesh. The double black row indicates the contribution of the element stiffness matrix that are taken into consideration at the global stiffness matrix. The dashed gray row shows the contributions that are outside the considered mesh and will not be computed. From the computational point of view, this procedures is equal to the one described for the 1D case.

**Boundary Conditions**. Figure 8 shows now the 7-atom chain with the boundary conditions. The dashed rows indicate the contributions that are not be taken into consideration in the assemblage of the global matrix.

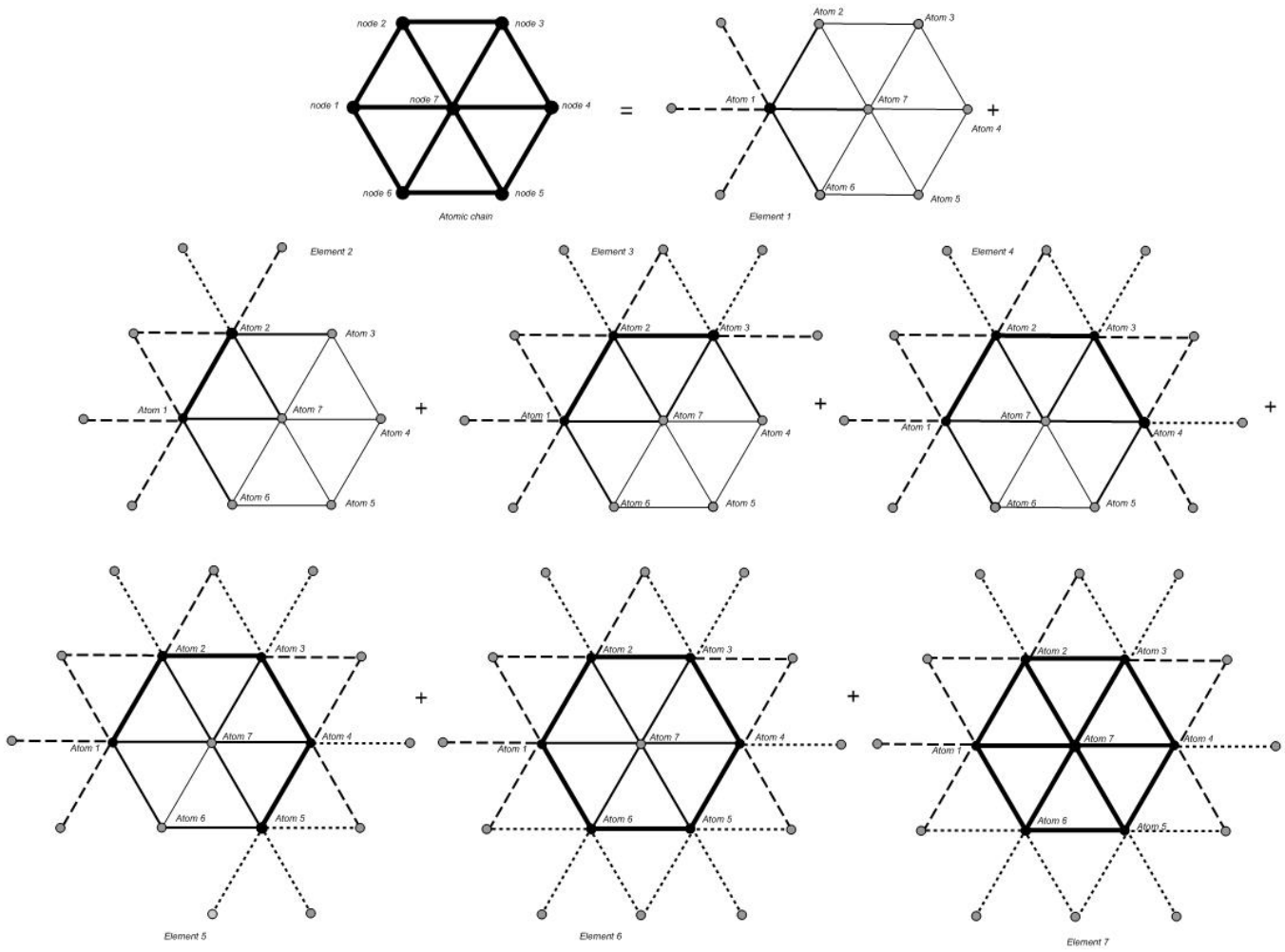


**Figure 7: Figure 7: Assemblage process for with a 7-node 2D AFEM**

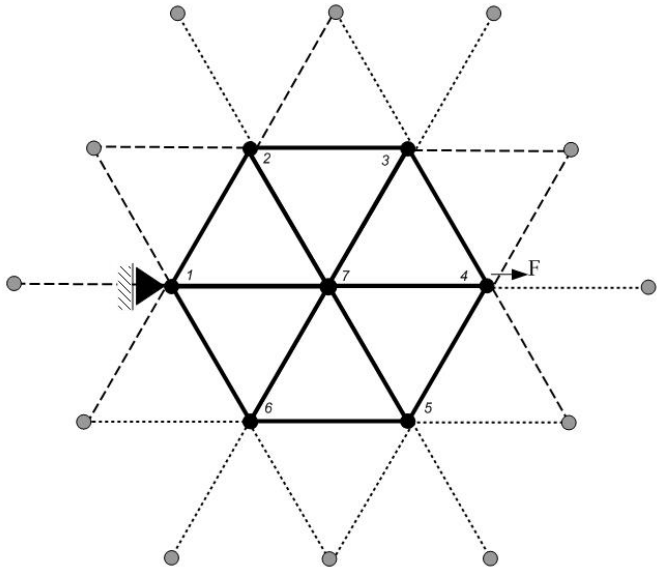


**Figure 8: A 7-node chain modeled with 7 elements.**

# 5 NUMERICAL RESULTS

**1D case.** As a basic example, a one dimensional atomic chain of 7 atoms, shown in Fig. 9 is analyzed. The atom number *1* is fixed and the atomic chain is excited by an external force *F*, applied on the atom number 7. To apply the AFEM, the total energy is calculated by using the Lennard Jones potential. In the present example the initial distance between two atoms is $r_{eq}$ = 1.12 Å. Three distinct AFEM elements, the 3-, 5- and 7-node elements, were used to model this 7-atom chain. In this example the force F is increased until the atomic chain fails.

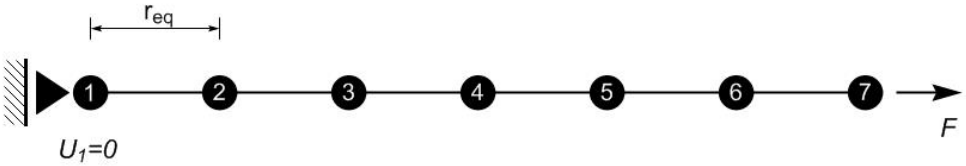


**Figure 9: A schematic diagram of a one-dimensional atomic chain**

The force-strain relations obtained with the present AFEM methodology is compared to simulation results obtained using the standard molecular dynamics (MD) code LAMMPS. The Lennard Jones potential were used at a temperature of 1 K. To simplify the Lennard Jones potential, $\sigma = 1$ and $\varepsilon = 1$. Non-periodic boundary conditions were used. The number of atoms, number of volume and temperature are constant. The time integration step for the MD simulation is 0.05 fs. For the MD simulations, three disctinc cut-off radius $r_c$ for Lennard Jones potential were set iqual to 1.5 Å, 2.5 Å and 3.5 Å, respectively. This corresponds to the 3-, 5- and 7-node elements of the AFEM simulation.

Considering $u_0$ the initial position and $u$ is the final position of a given atom, the strain is defined as:

$$\varepsilon = \frac{u - u_0}{u_0} \tag{27}$$

In all the following 1D results the force-displacement relations shown are those of atom 7 in the chain depicted in figure 9. Figure 10a shows the force-strain relation behavior obtained from AFEM using three disctinc cut-off radius $r_c$. A detailed view containing the last 4 load steps is shown in Fig. 10b. These figures show that there is very little difference between the results obtained with the 5-node and 7-node elements. On the other hand, Figures 10c and 10d show similar results obtained from the MD simulations. These results were obtained for three disctinct cut-off radius ($r_c$ = 1,5 Å; 2,5 Å and 3,5 Å), which emulate the distinct atomic scale elements. In this case there is also no noticeable difference between results obtained for $r_c$ = 2,5 Å and $r_c$=3,5 Å.

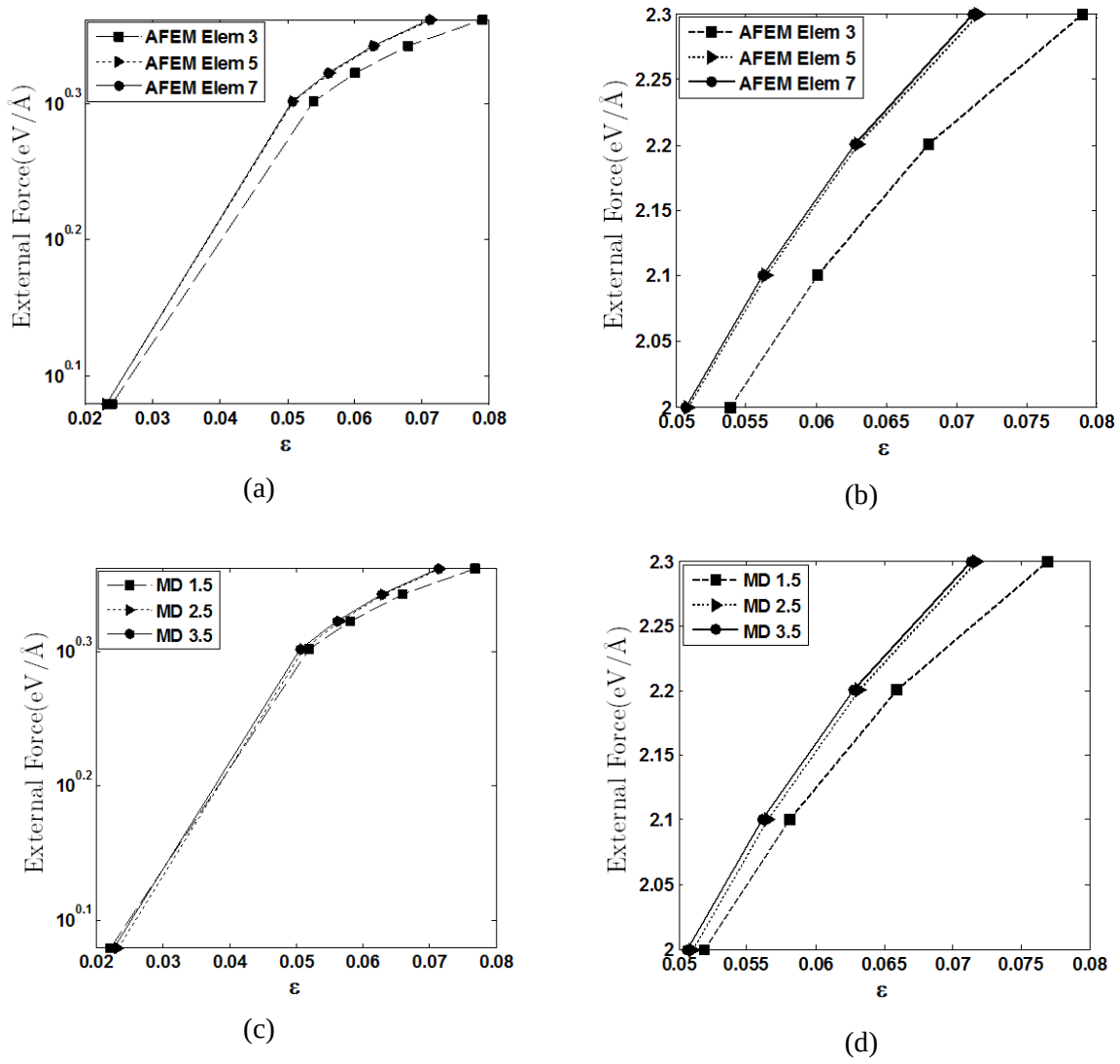


**Figure 10: (a)force-strain relation behavior from AFEM for the atom 7, (b) detailed view of Fig. 10a (c) force-strain relation behavior from MD for the atom 7, (d) detailed view of Fig. 10c.**

The results given above justify the fact that in MD simulations the cut-off radius is usually set equal to $r_c = 2.5\sigma$ (Smit, 1992). For the next numerical investigation for the MD simulation the cut-off radius is assumed to be $r_c = 2.5\sigma$. The next results show the role of the distinct atomistic elements (3- ,5- and 7-node) on the force-strain simulation. Figures 11a and 11b show the comparison of AFEM using 3-, 5- and 7-node elements and MD with $r_c$ = 2.5 Å. It can be seen that AFEM simulation using AFEM elements with 5 nodes is almost as accurate as AFEM using 7-node elements. A solultion for MD using $r_c$ = 2.5 Å is also presented in these figures.

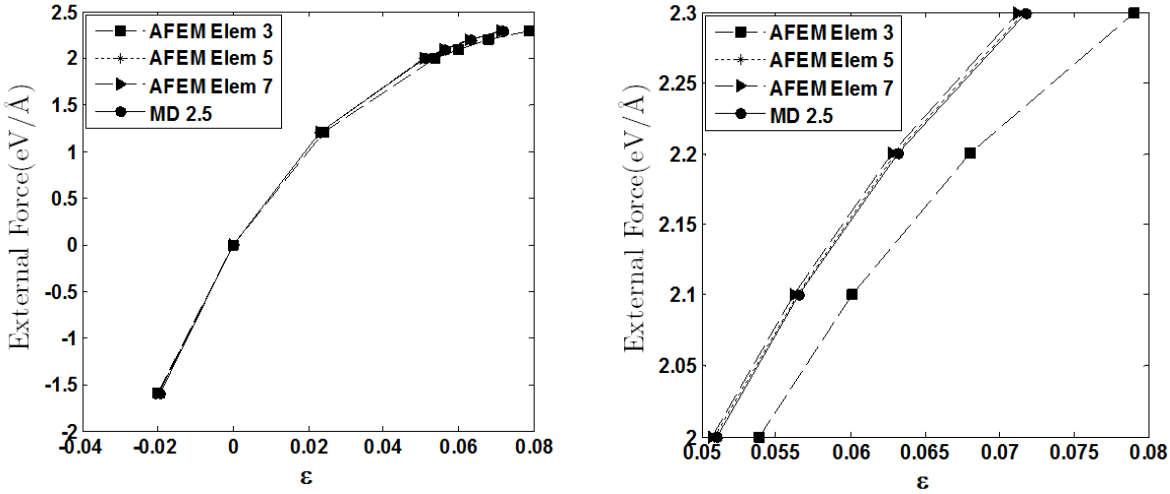


**Figure 11: comparison of AFEM using 3-, 5- and 7-node elements and MD with rc = 2.5 Å**

Figure 12a shows a force-strain relation from AFEM, using 5 node elements and MD, considering $r_c$ = 2.5 Å. Figure 12b shows relative error between these two solutions. It can be seen that there is a good agreement and that the relative error is usually less the $10^{-5}$, except near the zero force equilibrium position. The determination of this force-displacement relation is a non-linear procedure that must be solved iteratively. Figure 12c shows the number of iteration steps required to obtain a convergence within the error requirement that the $L_2$ norm of the non-equilibrium load vector is smaller than $10^{-11}$. For AFEM, this convergence requirement is obtained within $n_{it}^{AFEM} = 4$ and $n_{it}^{AFEM} = 8$ iterations. As the force and displacement increases, the number of iterations also increase in AFEM simulations. On the other hand, MD is also an iterative method and for this example needed $n_{it}^{MD} = 1000$ iterations to get a precision of 4 significant digits compared to the AFEM results. AFEM requires significantly less iterations to reach equilibrium within the same accuracy requirement of MD. Figure 12d shows the quantity u•P that is the dot product of the displacement vector by the non-equilibrium force vector, which can be viewed as a convergence measure of the AFEM results for the system at every iteration step (Kim, 2006).

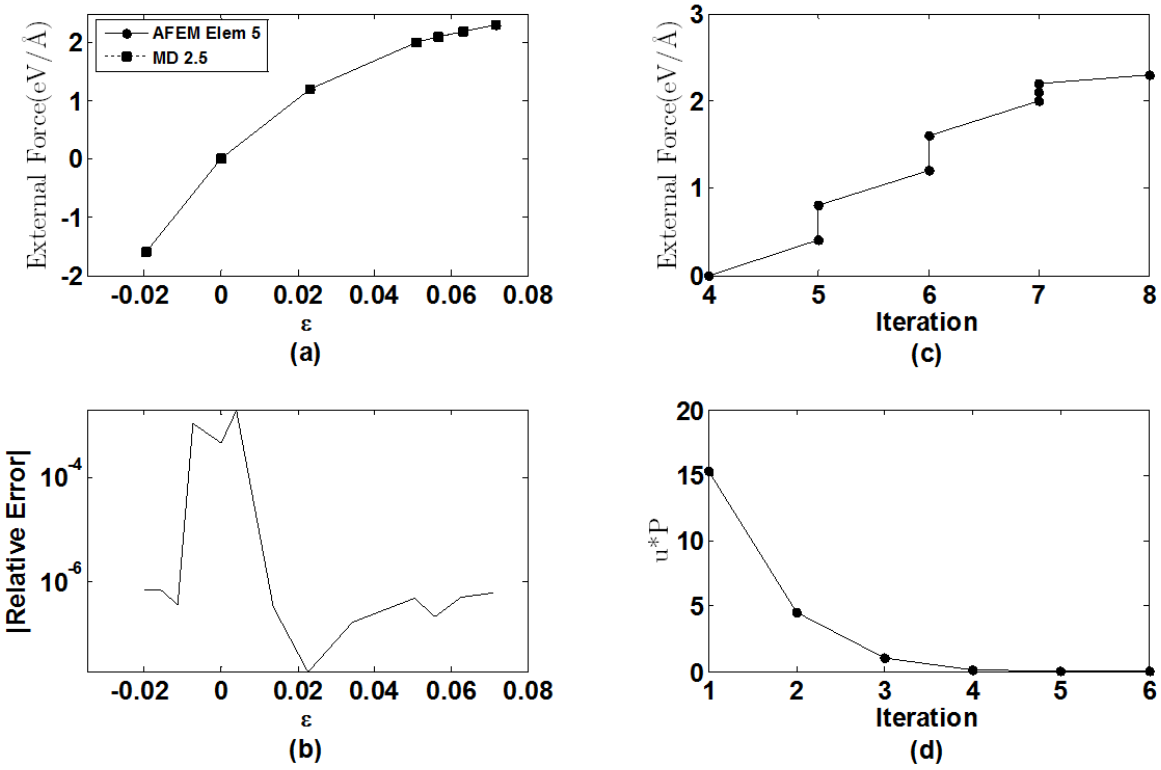


**Figure 12: force-strain relation; force by number of iterations, convergence relation and relative error**

**2D case**. As another example, a two-dimensional atomic lattice shown in Fig. 8 is analyzed. To build this atomic lattice 7 AFEM elements are necessary, as shown in Fig. 7. The atoms filled in black correspond to the complete AFEM element, and the atoms outside (in gray) correspond to the nodes, the contribution of which is not taken into account in assembling the global system stiffness matrix.

The boundary condition set on atom 1 was a constraint $u_1 = 0$, and the atomic lattice is excited by an external force *F* applied on the atom 4. The Lennard Jones potential were used at a temperature of 1 K. To simplify the Lennard Jones potential, $\sigma = 1$ and $\varepsilon = 1$. MD cut-off radius is set to 1.5 Å. Non-periodic boundary conditions were used. The number of atoms, number of volume and temperature are constant.

Figure 13a shows good agreement between AFEM and MD simulation, with relative error lower than $10^{-6}$ for the points far from equilibrium position ($u_4 \approx 0$) obtained for zero force ($F_4 = 0$), as shown in Fig. 13b. MD is an iterative method, and it took 1000 iterations to get into the final configuration with 4significant digits, when compared to the AFEM solution. On the other hand the AFEM simulation took a maximum of 7 iterations, as shown in Fig. 13c. Figure 13d shows the the quantity u•P that can be considered a measure of convergence of AFEM at every iteration step (Kim, 2006).

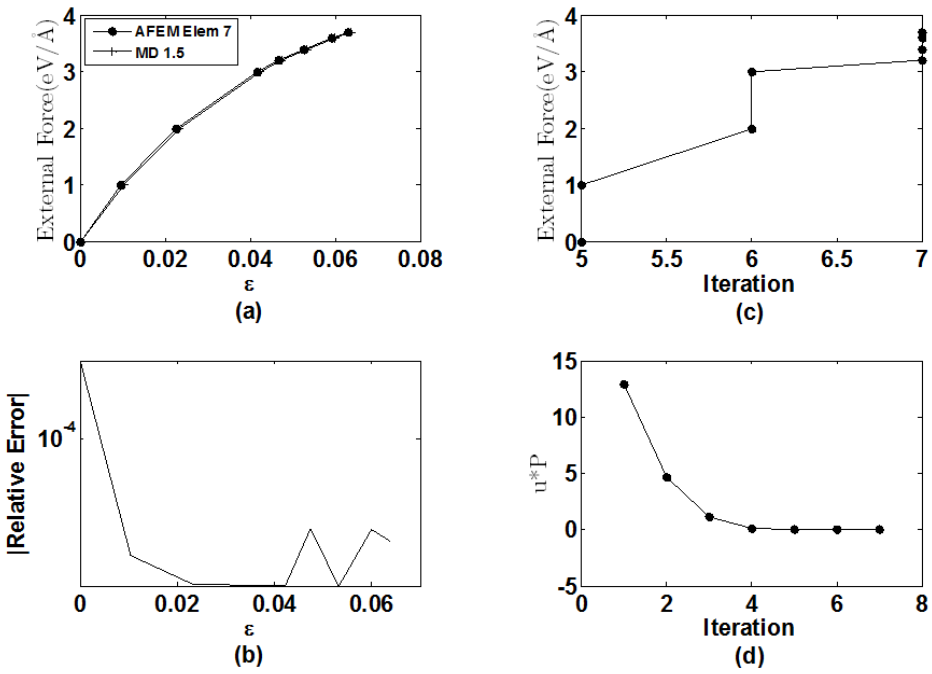


**Figure 13: Force-strain relation; force by number of iterations, convergence relation and relative error**

# 6 CLOSING REMARKS

In this article a formulation of the Atomic-scale Finite Element is revisited and implemented for the 1D and 2D cases to describe the atomic interactions described through the Lennard-Jones interatomic pair-wise potential. Explicit formulations for the stiffness matrices of the AFEM are given. Distinct atomic-scale elements with 3-, 5- and 7-nodes are described. The use of these elements is related to the cut-off radius assumed for the calculation of atomic interacting energy with the L-J potential.

The article shows how to assemble a global stiffness matrix based on the element matrices and how to disregard the element contribution of the nodes that are not present in the original atomic chain. Furthermore, the boundary conditions are incorporated in this scheme. From the programming point of view, the elimination of the stiffness contribution for the nodes that are not on the physical atomic chain is similar to introducing zero-displacement boundary conditions at one atom. Conceptually, nevertheless, the operations are completely different.

Simulations for a 1D atomic chain and for a 2D atomic mesh were conducted with the proposed non-linear AFEM and the results compared to those obtained from a classical Molecular Dynamics procedure based on the LAMMPS package (Plimpton, 1995). Force-strain curves were obtained for both cases and showed that for both, 1D and 2D simulations the AFEM procedure provides very accurate results. The number of iterative steps required for the non-linear AFEM and the corresponding MD simulations were examined. These results show that AFEM is much faster than the corresponding MD simulation, with the same precision requirements.

The proposed methodology could be extended to more complex interatomic potentials, like REBO (Brenner, 1990) or ReaxFF (Van et al., 2001), that can describe the mechanical behavior of nano-carbon structures and other complex nanostructures .

## ACKNOWLEDGEMENTS

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