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Dynamics of Macro–Nano Mechanical Systems; Fixed Interfacial Multiscale Method

M. H. Korayem*, S. Sadeghzadeh

Robotic Research Laboratory, Center of Excellence in Experimental Solid Mechanics and Dynamics, School of Mechanical Engineering, Iran University of Science and Technology, Tehran, I. R. Iran

(*) Corresponding author: hkorayem@iust.ac.ir
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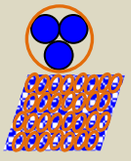
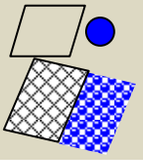
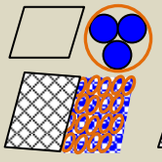
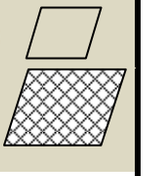
Abstract:
The continuum based approaches don't provide the correct physics in atomic scales. On the other hand, the molecular based approaches are limited by the length and simulated process time. As an attractive alternative, this paper proposes the Fixed Interfacial Multiscale Method (FIMM) for computationally and mathematically efficient modeling of solid structures. The approach is applicable to multi-body mechanical systems. In FIMM, a direct link between the nano field atoms and macro field nodes by the local atomic volume displacements associated with every macro field node in their common zone has been replaced with the previous methods. For a complete model of the macro section, a nine-noded Lagrange element has been developed, and for small dimensions, the Sutton-Chen potential (for problems of mechanics) has been used. In the presented model, the undesirable effects of free surfaces, common surfaces, and surfaces close to the interface with the macro field have been eliminated, and after presenting a practical and noteworthy procedure for the dynamics of systems in general, seven problems (in the form of three examples) have been offered to showcase the practicality, simplicity, and the effectiveness of this method.
Keywords: *Multi-scale model; Open systems; Dynamics; Macro/nano mechanics; coupling model, FIMM.*

1. INTRODUCTION

Although they have been extensively applied for simulation of large scales, the continuum mechanics-based methods, including the finite element or other numerical methods, don't provide the correct physics in atomic scales. Table 1 lists a complete span of various scales and models in material modeling. Upon the appearance of advanced technologies, the interfacial behavior of macro (large) to nano (small) scales has been discussed. Connectivity of models in various scales was the first and the best approach of course. This approach named Multiscale method and has been studied and developed in a lot of works for various systems. In multi-scale approaches, implementation of molecular based models guarantees the correctness of obtained behavior in small scales; while for larger dimensions that don't have tangible nonlinear behavior, utilization of continuum mechanics (CM) based methods is effective, and there is no need to spend a lot of time by application of the atomic models for these parts. Therefore, the continuum mechanics models and the atomic models interact with each other in such a way as to model the whole system and achieve the goal which has been defined and set.

During the last decades, a lot of efforts have been conducted to provide the numerical solutions for macro field. As was pointed out in the previous section, the common conventional models have many limitations. Despite their reasonable computational costs, the continuum mechanics methods are totally incapable of describing phenomena in the nano scale. On the hand, molecular dynamics models are very limited with respect to the time dimension; as the modeling of objects in the micrometer and

Table 1: *A complete span of various models in material modeling*

Length Scale	**Sub atomic**	**Nano**		**Micro**		**Macro**
Time Scale	Sub nano Sec	Nano Sec		Micro Sec		**Sec**
Theory→	Small scale approaches	Multiscale approaches				Large scale approaches
Features↓	Quantum Mechanics	MD	SCGMD	CM-MD coupling	CM-SCGMD coupling	Continuum Mechanics (CM)
Structure unit	Phonons	Atom	Site	Element-Atom	Element-Site	Element
Unit Shape						
System Shape						
Lattice Deformation	Discrete	Discrete	Discrete	Continuous-Discrete	Continuous-Discrete	Continuous
Time Scale	Below 1pSec	1fSec-1nSec	1fSec-1μSec	1nSec- 1 mSec	1nSec-1Sec	1mSec-several hours
Length Scale	1fm-1A□	1A□ - 10nm	1fm-100nm	1nm-10μm	1nm-1mm	1μm-several meters
Applicable to	Sub atomic studies	Molecular sciences	Nano to micro Medicine	NEMS, Nanorobotics, manipulation, drug delivery	Nanorobotics, MEMs, NEMS	Macro scale systems
Not applicable to	Super nano metric systems	Macro processes in long duration	Super micro processes with large time scales	Molecular sciences and sub atomic studies	Molecular sciences and sub atomic studies	Small, huge and non homogeneous systems

microsecond dimensions is only possible by means of supercomputers. So, researchers are trying to use the advantages of the aforementioned methods and to overcome the existing flaws by combining them together. The outcome of these efforts has been the development of multi-scale methods.

Multi-scale methods are divided into "hierarchical" and "concurrent" groups. In the hierarchical models, the properties are calculated at one scale and then passed on to another scale. In other words, the information obtained from one model is enriched by another model. These approaches include two groups, in which, the information from micro-scale systems is transferred to the continuum mechanics model. The first group are the models based on the Cauchy-Born hypothesis [1, 2], in which, the information acquired from the atomic structure of the object clearly reveal themselves in the calculation of the elastic stress and tensor of the material's properties. The second group of these models is based on the Virtual Atom Cluster (VAC) [3], in which, the structure of the material is enriched on the basis of the information obtained from molecular mechanics. This method has been used for the study of carbon nano tubes.

In the concurrent models, there are several simultaneous models in the multi-scale simulation, and information is exchanged among them concurrently. These methods are the result of efforts that have tried to combine the molecular dynamics models with the continuum mechanics models. Over the past decade this group of multi-scale models has received considerable attention in the literature. It includes various frameworks, but

three major methods may be addressed. The quasi-continuum method [4, 5], which was presented by Ortiz et al., is now the most applied method, and many studies have been conducted on this method. The other model is the Bridging Domain method [6], which has been developed by Belytschko et al. In this method, in part of the simulation zone, the continuum domain and the atoms exist together; therefore, the validity of this model in the bridging domain needs to be investigated extensively. The third approach, known as the Bridging Scale method [7, 8], has been presented by Liu and his colleagues. In this method, it is assumed that the continuum solution is not exact and the resulting error can be removed through molecular dynamics. The most important issue in the development of these hybrid methods has been the formulation of a comprehensive computational coupling along the interface.

This fact has been revealed in a brief review of the developed and presented methods. In the coupling models, the continuity of the material's characteristics should be preserved during the transition from the atomic forces to the stress-strain field of continuum mechanics. Coupling models have been developed for many problems, including the crack problem, and they have often been named Finite Element–Atomistic (Feat) coupling procedure, which is the combination of molecular dynamics and finite element models. Likewise, a general formulation of the ordinary finite element, which allows the Macro Field (MF) nodes to be examined as coarse and fine Nano Field (NF) atoms, has resulted in another computational scheme for the coupling of the continuum and the atomic environments, called the Coarse-Grained Molecular Dynamic (CGMD).

The Quasi-Continuum (QC) method that has been studied by Miller and Tadmor [9] is explicitly based on the complete description of a material's environment. The Coupled Atomistic/Dislocation Dynamics (CADD) method of Shilkrot et al. [10] has been presented for the simulation, detection, and justification of the separations between the atomic and the continuum regions. This model had first been offered for the simulation of materials at zero degrees Kelvin (0 K), but recently, it has been developed to deal with the effects of finite temperature as well.

The general characteristic of these approaches, for the atomic and continuum coupling, has been the fine-graining and manipulation of MF mesh configuration for conformity with atomic length scales, and also the kinematic coupling of finite element nodes to discrete atoms along an interface. Henceforth, the approaches that make a one to one coupling between the atoms and finite element are called Direct Coupling (DC).

When DC procedures are followed, the major problem that arises is the inherent difference between the atomic and the continuum computational models. The physical state of the atomic region is described by means of the non-local inner-molecular forces between discrete atoms with specific position and moment; while the physical state of the continuum region is described by using the stress-strain fields which are statistical averages of the atomic attractions at larger scales of length and time. Generally, the ordinary coupling between discrete and continuum values can only be obtained by taking a statistical average of the scales in which the discreteness of the atomic structure can be approximated in the quasi-continuum form. Although, much better ways could be offered for the development of methods of coupling of the continuum domain with discrete domain, nevertheless, the application and development of these methods for the static and dynamic problems related to mechanical engineering is highly important.

Up to now, the FEM was the most applied approach for macro part of coupling models; while, much better and more accurate methods, and even more exact numerical methods, exist for this purpose. Thus, in describing the problem, instead of the finite element method, the more general form of finite element, i.e. the MF solution method, is used. Based on this notion, we try to present a model that can be attached to the finite element method without any restriction, and can be used with other methods as well.

So far, various NF-MF coupling frameworks have been presented. The work of Park and Liu [11] is an attempt to describe the multiscale method ideas and capabilities in the field of solid structures. Recently, some concentrated groups have focused on the multiscale approaches for various applications. They introduced various frameworks with capabilities of application to solid structures. For instance, Macroscopic Atomistic

Ab initio Dynamics (MAAD) method [12, 13], Heterogeneous Multiscale Method (HMM) [14], Multiscale Field Theory (MFT) [15] and Embedded Statistical Coupling Method (ESCM) [16] may be addressed.

In this paper, a Fixed Interfacial Multiscale Method (FIMM) is proposed for computationally and mathematically efficient modeling of solid structures. The approach is applicable to multi-body mechanical systems. In FIMM, a direct link between the nano field atoms and macro field nodes by the local atomic volume displacements associated with every macro field node in their common zone has been replaced with the previous methods.

Moreover, considering the mechanics of the problem, and using a system of equations in matrix form, a dynamic algorithm has been presented for dynamically solving the problem. The macro and nano field's computational systems are independent of each other and only relate through an iterative update of their boundary conditions. This method presents an improved coupling approach which is inherently applicable to three-dimensional domains. In addition, it prevents the resolving of the continuum model into atomic resolution, and allows finite temperature cases to be applied. One of the prominent features of the present work is the presentation of reliable solutions for problems that include natural, forced, body, and interfacial degrees of freedom. Since solids are fairly rigid at the macro zone, the interfacial volume of the considered system has been moved to macro part and then, it assumed to be rigid.

Thus, FIMM leaves negligible relative motion of atoms in every atomic volume by moving the interface into the macro part. Now, previous nano field and a bit of macro part form the new nano field. This leads to larger dimensions for nano field with regard to the last one. One major difference between ESCM and FIMM is the constraint of coupling, where ESCM uses a local average of atoms included in an interfacial volume.

In the following, both the macro (continuum model) and nano (atomistic model) field theories are discussed briefly first. Then, FIMM has been presented in details and validated by comparison with MD, CGMD, ESCM and MAAD approaches for a clamped silicon wafer in plane strain condition. At the end several useful results and discussion have been introduced

2. AN OVERVIEW OF FEM AND MD

Extensive work has been done on the development of Finite Element Method for various systems. Since in mechanical systems, usually the macro section has a moving part and a sensing part, and these parts often operate by means of the piezoelectric property, we try to deal with the macro section from this perspective. Rajeev kumar et al. [17] investigated a finite element model for the active control of induced thermal vibration in layered composite shells with piezoelectric sensors and actuators (piezothermoelastic). Then, they presented a finite element formulation for the modeling of static and dynamic responses of multi-layered composite shells with integrated piezoelectric sensors and actuators, and subjected to mechanical, electrical, and thermal loadings [18].

In 2008, Zia et al. [19] have presented a finite element formulation for the vibrations of layered piezoceramic plates, which accounts for the effects of hysteretic behavior. The hysteretic behavior has been simulated in the dielectric domain by using the finite element method and applying the Ishlinskii's model. In 2008, Balamurugan and Narayanan [20] have used a nine-noded piezolaminated degenerated shell element in order to model and analyze multi-layered composite shell structures together with sensors and piezoelectric actuators.

The coordinates of any arbitrary parameter, at any arbitrary point can be expressed by the use of nodal coordinates and isoparametric shape functions in the following way

$$\boldsymbol{\mathcal{P}} = \sum_{i=1}^{Q} \aleph_i (\xi, \eta, \zeta) \boldsymbol{\mathcal{P}}(X_i) \qquad (1)$$

Where $\boldsymbol{\mathcal{P}}$ is the noted parameter, $\aleph$ is the isoparametric functions, Q is number of nodes of the considered element, and X is the position of the nodes. By using the kinetic, potential and external energies and writing the minimum energy principle, the equations of motion for the finite element system can be presented as:

$$\left[M_{uu}\right]_e \ddot{q}_e + \left[C_{uu}\right]_e \dot{q}_e + \left[K_{uu} - K_{u\phi} K_{\phi\phi}^{-1} K_{\phi u}\right]_e q_e = F_{qe} - \left[K_{u\phi} K_{\phi\phi}^{-1}\right]_e F_{\phi e} \qquad (2)$$

where $[M_{uu}]_e$, $[K_{uu}]_e$, $[K_{u\phi}]_e$, F_{qe}, $[K_{\phi\phi}]_e$, $F_{\phi e}$, $[C_{uu}]_e$, and q_e are respectively, the element's mass matrix, stiffness matrix, electromechanical coupling hardness matrix, mechanical load, dielectric hardness matrix, electric force vector, structural damping matrix, and the vector of change of degrees of freedom in the considered system.

In MD, a well defined potential function $U(r_1, r_2, \ldots, r_N)$ expresses the manner of dependency of the potential energy of a system consisting of *N* atoms with the space coordinates $r_1, r_2, \ldots, r_N$. The equation of motion of all atoms model can be expressed as

$$m_i \ddot{r}_i = -\nabla_i U + F_i \tag{3}$$

Where, m and F are the mass of atoms and external (boundary) forces. The Finite Difference Method (FDM) is the usual approach for solving the differential equations of motion. FDM includes various approaches for analyzing the problem. Verlet and Velocity Verlet algorithms are the most famous methods. These algorithms are combination of the forward and backward Taylor expansions [21].

In addition to the Lenard Jones potential as a famous one, the Embedded Atom Potential (EAM), Finnis-Sinclair potential [22] and Sutton-Chen potential [23, 24] may be addresses as multi-particle potentials. They may be implemented in the simulation of solid structures as well as the bio and fluidic fields. However, the solid structures are especial nano fields that mentioned potential should be improved for better results. The Rafii-Tabar-Sutton multi-body long-range potential is used in the current study which is an extended and improved form of Sutton-Chen potential with the capability of modeling the unlike material's interactions. The general form of Rafii-Tabar-Sutton (RTS) potential for binary A-B unlike materials is [23 , 24]:

$$H_I^{RTS} = \frac{1}{2}\sum_i \sum_{j\neq i} V(r_{ij}) - d^{AA}\sum_i \hat{p}_i \sqrt{\rho_i^A} - d^{BB}\sum_i (1-\hat{p}_i)\sqrt{\rho_i^B} \tag{4}$$

With

$$V(r_{ij}) = \hat{p}_i \hat{p}_j V^{AA}(r_{ij}) + (1-\hat{p}_i)(1-\hat{p}_j) V^{BB}(r_{ij}) + \left[\hat{p}_i(1-\hat{p}_j) + \hat{p}_j(1-\hat{p}_i)\right] V^{AB}(r_{ij}) \tag{5}$$

$$\rho_i^A = \sum_{j\neq i} \Phi^A(r_{ij}) = \sum_{j\neq i}\left[\hat{p}_j \Phi^{AA}(r_{ij}) + (1-\hat{p}_j)\Phi^{AB}(r_{ij})\right] \tag{6}$$

$$\rho_i^B = \sum_{j\neq i} \Phi^B(r_{ij}) = \sum_{j\neq i}\left[(1-\hat{p}_j)\Phi^{BB}(r_{ij}) + \hat{p}_j \Phi^{AB}(r_{ij})\right] \tag{7}$$

Where $\hat{p}_i$ is the site occupancy operator and defined as:

$$\hat{p}_i = \begin{cases} 1 & \text{if site i is occupied by an A atom} \\ 0 & \text{if site i is occupied by an B atom} \end{cases} \tag{8}$$

The functions $V^{xy}(r)$ and $\Phi^{xy}(r)$ are defined as

$$V^{xy}(r) = \varepsilon^{xy}\left[a^{xy}/r\right]^{n^{xy}} \tag{9}$$

$$\Phi^{xy}(r) = \left[a^{xy}/r\right]^{m^{xy}} \tag{10}$$

And the constants are defined by

$$d^{AA}=\varepsilon^{AA}C^{AA} \qquad d^{BB}=\varepsilon^{BB}C^{BB}$$

$$m^{AB}=\frac{1}{2}(m^{AA}+m^{BB}) \qquad n^{AB}=\frac{1}{2}(n^{AA}+n^{BB}) \quad (11)$$

$$a^{AB}=\sqrt{a^{AA}a^{BB}} \qquad \varepsilon^{AB}=\sqrt{\varepsilon^{AA}\varepsilon^{BB}}$$

Where ε is a parameter with the dimensions of energy, 'a' is a parameter with the dimensions of length and is normally taken to be the equilibrium lattice constant, 'm' and 'n' are positive constants with n>m. This potential has the advantage that all the parameters can be easily obtained from the Sutton-Chen elemental parameters of metals [24].

In a lot of existent mechanical systems, the small field includes a large area with respect to the atomic dimensions. For instance, in nanorobotic devices, the nano filed includes some nano and some micro parts. So, MD could not cover the simulation of nano field alone, yet MD may be modified to apply in larger sizes (with limitations in the aspect ratio). Clustering the all atom MD model into a coarse grained site model, named Coarse Grained MD (CGMD), is a simple and effective method for this purpose.

3. COARSE-GRAINED MOLECULAR DYNAMICS

Electromechanical processes normally occur on the order of nano, micro, milli, and even several seconds. In addition, they have higher-than-nano dimensions. Therefore, their real dimensions and time ranges cannot be determined through the use of molecular dynamics method. However, by the use of "coarse graining", larger dimensions, in longer time ranges could be modeled.

Now, since a remarkable method by the name of Coarse-Grained Molecular Dynamics (CGMD) has been presented for this purpose, while using it here, a general description is also provided regarding this approach. The CGMD method is based on the notion that, if instead of one atom, a larger number of atoms are taken as a unit, then, a larger volume of material and also more simulation time can be considered. Even by utilizing the world's largest and most advanced supercomputers, the molecular dynamics simulations cannot be performed for more than several microseconds. Various approaches have been presented for the CGMD methods [21-23].

The only crucial issue in these models will be the manner of predicting and estimating the system's potential. Achieving a good potential for the system can be guaranteed through a dimension analysis, and by comparing the Radial Distribution Function (RDF) of the system with obtained CGMD in the NF process; although, other ways also exist for this achievement. If, on the average, the nominal mass and distance of atoms are on the order of $'m_c'$ and $'L_c'$, and the nominal mass and distance of the CGNF samples are on the order of 'm' and 'L', respectively, the following relations could be considered for the time steps that are used:

$$\Delta t_{max}\big|_{MD} \sim L\sqrt{\frac{m}{kT}} \quad \text{and} \quad \Delta t_{max}\big|_{CGMD} \sim L_c\sqrt{\frac{m_c}{kT}} \quad (12)$$

We developed a new CGMD approach and validated it with proper results [25, 26]. It has been utilized in this paper for the NF.

4. MACRO-MICRO COUPLING MODEL

To generalize the problem, the macro-nano-related problems are divided into two groups of closed and open systems. The group of problems, where all the side boundaries of the nano domain overlap the interfacial degrees of freedom, are called "closed systems"; and the group of problems, where the side boundaries of the nano region, in addition to the interfacial degrees of freedom, possess limited (and in some cases, unlimited) degrees of freedom, are called "open systems". Figures 1 and 2 illustrate the general cases of the closed and open systems, respectively. In the closed system, usually one nano field and one macro field exist. For example, in the crack propagation problem, the fine region of crack propagation is designated as the nano field, and the coarse region in which the crack is growing is designated as the macro field. In the open system, several macro fields could be interacting with several nano fields. If the numbers of macro and nano fields are equal to M and N, respectively, and

the area of each field is indicated by Ω, then for the closed system, we can write:

$$\begin{cases} \Omega_i \cap \Omega_j = \varnothing, & i,j \in NF \\ \Omega_i \cap \Omega_j = \prod or\, \varnothing, & i,j \in MF \\ \Omega_i \cap \Omega_j \neq \varnothing, & i \in NF,\quad j \in MF \end{cases} \tag{13}$$

And for the open system:

$$\begin{cases} \Omega_i \cap \Omega_j = \prod or\, \varnothing, & i,j \in NF \\ \Omega_i \cap \Omega_j = \prod or\, \varnothing, & i,j \in MF \\ \Omega_i \cap \Omega_j = \prod or\, \varnothing, & i \in NF,\quad j \in MF \end{cases} \tag{14}$$

In the above relations, $\varnothing$ and $\prod$ denote the empty and non-empty spaces, respectively. With this notation, it can be easily proved (considering the presented definitions) that a closed system is a special case of an open system. Therefore, in an open system, there may be more than one nano field and each of the nano fields may be in contact with one another in different ways.

These contacts (for example in the nanomanipulation process using nanorobots) may not occur during a certain time range, and after that duration, these contacts may be established. Exclusively mechanical systems are taken into account, and therefore, the mentioned contacts are of the second order only, and volumetric sharing is not considered.

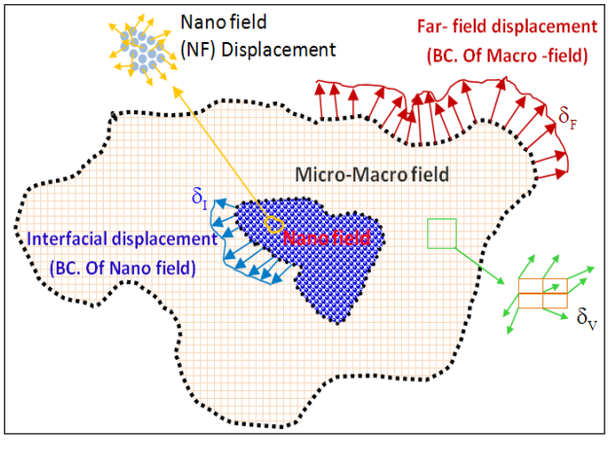


Figure 1: *General case definition of closed mechanical systems*

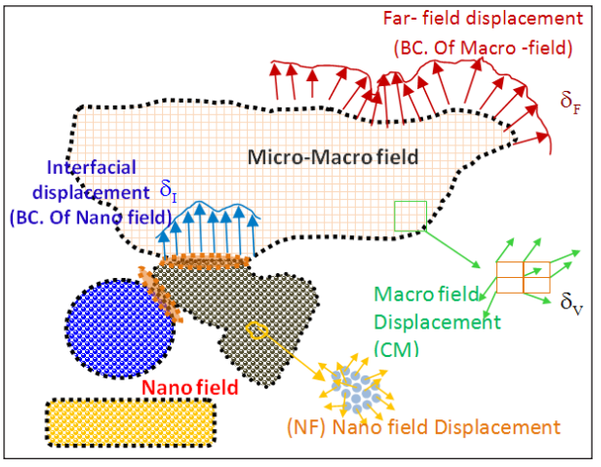


Figure 2: *General case definition of open mechanical systems*

The concept of multi-scale coupling methods can be very useful in cases where we want to model a relatively large region of the material in order to study the whole deformation field, but the atomic and sub-atomic scales are needed only in specific and limited regions. A practical example of a closed system can be demonstrated in the modeling of crack nucleation and propagation. As was mentioned before, for such problems, various works have been presented.

The present model has a special application in open systems; systems where practically no interface may even exist between the macro and nano environments in some cases and in a certain range of work, while after a certain time duration (which could be known or unknown), a relationship may form between these two environments. Through the use of coupling models for closed environments, the size limitation of atomic modeling could be minimized, such that an inner region (with complex dynamic processes and large deformation gradients) could exist inside an outer region (with small deformation gradients). It is not like this in open systems, where the effect of size will be considerable. To demonstrate the effectiveness of the model, in this article, the special case of a conic region for NF has been investigated. Also, in the MF model, an elastic beam with piezoelectric properties has been considered.

4.1. Coupling of MF and NF

For the coupling of MF and NF in closed

systems, four regions are considered throughout the system shown in Figure 3. These four regions, in the order of proceeding from micro to nano environments, consist of: Macro Field (MF), Unfolded Volume (UV), Interfacial Volume (IV), and Nano Field (NF). The IV region is in fact a region where the terminal atoms of a NF model have surrounded a MF node in the model. The IU region is the region between the end nodes of MF and the end of the NF model. The two regions of MF and NF need no further explanation. In view of the presented cases, IVs estimate the mean displacements of NF in the center of mass of these displacements. These averages are later used as the initial conditions of displacements in the relevant interfacial nodes. It should be mentioned that, the IV need not match the macro element that surrounds it, with respect to the size and shape. Normally, a macro element, in the interfacial section, consists of hundreds to thousands of atoms. By taking an effective average for the atomic points, the discreteness of the atomic structure can be sufficiently homogenized so that the MF region responds to the excitations of the atomic region as an expanded volume of itself.

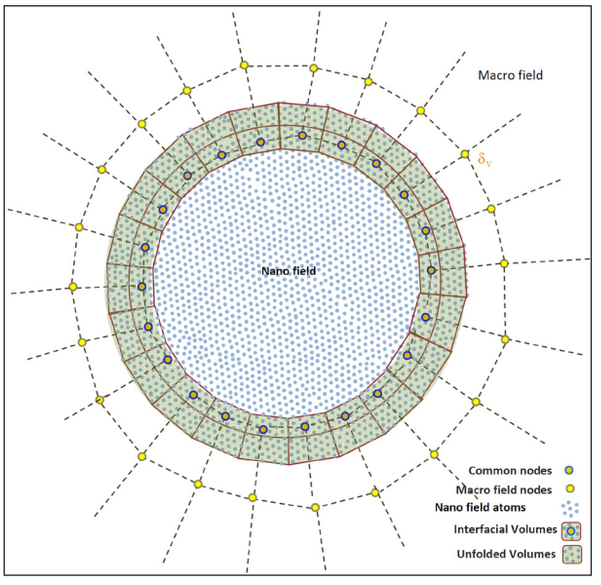


Figure 3: *Common region between NF and MF in the closed system*

For the analysis of open systems, in addition to the four regions of MF, UV, IV, and NF, two regions of Free Boundaries of nano field (denoted by FB)

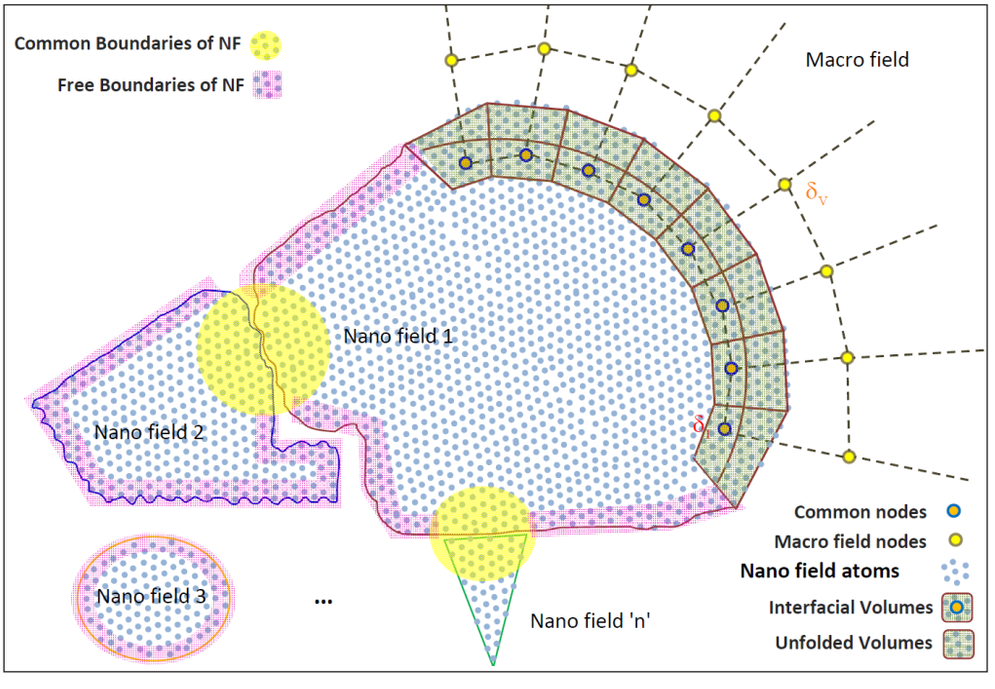


Figure 4: *Common region between NF and MF in the open system*

and Common Boundaries of nano field (denoted by CB) are also defined (Figure 4). Regardless of the type of initial state these two regions may have, each one has the potential of undergoing different changes during the analysis time range. The CB region is usually circumscribed around a circular zone, because in small dimensions, for considering the forces which in this zone are accounted among different sections of the nano field, the concept of "cut off radius" is used. Moreover, the MF region is also divided into four sections of "free far-fields", "internal volume", "boundary field", and "interfacial field".

It seems necessary here to describe the method of analysis of the FB and CB regions. In order for the FB region to behave freely (at surface), changes should be made to the model. This is the philosophy behind the establishment of the FB region. The existence of free surface creates unwanted effects in the NF system.

In comparison with the cases in which the boundary is affected by an external load, this occurrence in FB is not so critical. In addition to unwanted effects, since atoms at the free surface or close to it don't have a complete set of neighboring atoms, the coordination between the atoms falls apart. To remedy this lack of coordination, and to make the atoms stable in the interfacial NF region, two approaches can be adopted. The first approach is to offer an additional volume of atoms away from the center, which forms the surface NF region. The second approach is to consider a number of the same NF system atoms as an unfolded volume.

In case of using the first approach, although the surface NF region eliminates the effects of the free surface, it applies an unwanted virtual stiffness to the system, which elastically constrains the deformation of the inner NF region. To counteract this effect, the unwanted virtual hardness should be compensated. Since the effects of surface in solids are controllable, to a large extent, by the inner volume, in this article, it is suggested to use the second approach. Of course, in places where the limitation of size exists (like the tip of a cone-shaped region), the use of the first approach is inevitable.

During the simulation, the average of k numbers of IV, for obtaining the displacement of the center of mass is defined as $\vec{\delta}^{MD}_{CM,k}$, which, to get the statistical displacement vector $\vec{\delta}^{MD}_{I,k}$, is averaged along M time ranges of NF:

$$\vec{\delta}^{MD}_{I,k} = \left\langle \vec{\delta}^{MD}_{CM,k} \right\rangle_{Time} = \frac{1}{M}\sum_{j=1}^{M}\left(\vec{r}_{CM,k}(t_j) - \vec{r}_{CM,k}(0)\right) \tag{15}$$

In the above relation, $\vec{r}_{CM,k}(t_j) = \frac{1}{N_k}\sum_{i=1}^{N_k}\vec{r}_i(t_j)$ is center of mass of the k[th] IV, which has N_k atoms in the position $\vec{r}_i$ at time t_j of the j[th] NF time range. In open systems, in order for the NF region to behave freely (at surface) or to be subjected to specific external forces, some alterations should be made in the model. This is the philosophy behind the establishment of the UV region. In the best case, when the free movement of the surface is intended, the existence of the free surface produces unwanted effects in the NF system.

This event, in cases where an external force is considered instead of the free movement, will be much worse. In addition to unwanted effects, since atoms at the free surface or close to it don't have a complete set of neighboring atoms around them, the coordination between the atoms falls apart.

To reduce this lack of coordination, and to make the atoms stable in the interfacial NF region, an additional volume of atoms far from the center, which forms the surface NF region, is offered. On the other hand, although the surface NF region eliminates the effects of the free surface, it applies an unwanted virtual stiffness to the system, which elastically constrains the deformation of the inner NF region. Due to the particular complexity of the problem, in this report, a simple, and at the same time, effective procedure is presented for the calculation of virtual hardness.

4.2. Algorithm for establishment of coupling

In general, the coupling of MF and NF is accomplished through schemes based on the establishment of iterative equilibrium between these two regions. In these schemes, the iterations begin with the displacements of the MF and NF interface. These displacements are obtained as statistical average from the atomic positions of every IV, and by averaging in the time duration of NF. These average displacements are then applied in the MF region, as displacement boundary conditions ($\vec{\delta}_I$). Then, the obtained MF boundary value problem is solved to yield the new interfacial reaction forces,

i.e. $\vec{R}_I$. Then, these forces are applied to the atoms located in IVs; and so, the fixed-reaction boundary conditions are defined in the NF system. During the iterations in which MF is solved, the reaction boundary conditions are fixed, and they are applied to the NF region to guarantee the correct application of the elastic field from the MF domain. In solving the problems of statics, the iteration cycle of NF and MF continues until the system reaches a lasting equilibrium of displacements and forces between the continuum and atomic fields. While for the problems of dynamics, after the establishment of static equilibrium (using the aforementioned method), the system should be dynamically solved (generally via numerical methods). This issue constitutes one of the substantial complexities of the present work.

Here, through a unique algorithm, the manner of analysis of mechanical dynamic problems will be presented. By considering the dynamics in the MF model, dynamic continuum equations in the nth MF step at time t_n are given as:

$$\mathcal{C}(\mathfrak{p}(t_n),\dot{\mathfrak{p}}(t_n),\ddot{\mathfrak{p}}(t_n),...)=\mathfrak{R}(t_n) \tag{16}$$

where $\mathcal{C}$ is the term related to the equations extracted from the system's internal energy, which in different methods, are functions of $\mathfrak{p}(t_n)$s (the studied variables of the system) and of different orders of their derivatives. Also, at different times, function $\mathfrak{R}(t_n)$ is the function resulting from external loads applied to the system and proportionate to the orders of the system.

In problems that possess natural and forced boundary conditions and, at the same time, are supposed to be used in multi-scale coupling models, the degrees of freedom should be divided into several groups. The first group includes the degrees of freedom that are governed by the natural boundary conditions. This group will be designated by F. The free boundary condition is the most usual condition of this group. The second group includes the degrees of freedom that are governed by the forced boundary conditions. This group will be designated by B. In many problems related to dynamics of solids, the clamped boundary condition can be regarded as a forced boundary. Also, in the area of fluid dynamics, the no-slip conditions at the surface can be mentioned. The third group is the degrees of freedom that are included in the inner points of the domain.

This group will be designated by V. The fourth group is the degrees of freedom that are supposed to be coupled with the common degrees of freedom in molecular dynamics. This group will be designated by I. The matrices related to the degrees of freedom of general equation (1) are reduced, based on these definitions.

Therefore, $\mathcal{C}$ is broken down as $[\mathcal{C}_{\alpha\beta}]$, in which $\alpha,\beta=V,F,I,B.$ V indicates the internal MF region, F is the far-field variables, I is the variables of the interface, and B is the variables of the MF boundary conditions. Using these definitions, the dynamic continuum equations in the nth step of MF at time t_n are expressed as:

$$\mathcal{C}_{\mathfrak{f}}(\mathfrak{p}(t_n),\dot{\mathfrak{p}}(t_n),\ddot{\mathfrak{p}}(t_n),...)=\mathfrak{R}_{\mathfrak{f}}(t_n),\quad \mathfrak{f}=V,F,I,B \tag{17}$$

It should be noted here that $\mathfrak{p}(t_n)$ includes all the degrees of freedom in every set of equations. The general state of a multi-scale problem includes the initial value and the external forces problems.

4.2.1. Initial value problem

The general equations of motion of the macro system's displacement, when no external forces exist, are as follows:

$$\mathcal{C}(\mathfrak{p}(t_n),\dot{\mathfrak{p}}(t_n),\ddot{\mathfrak{p}}(t_n),...)=0 \tag{18}$$

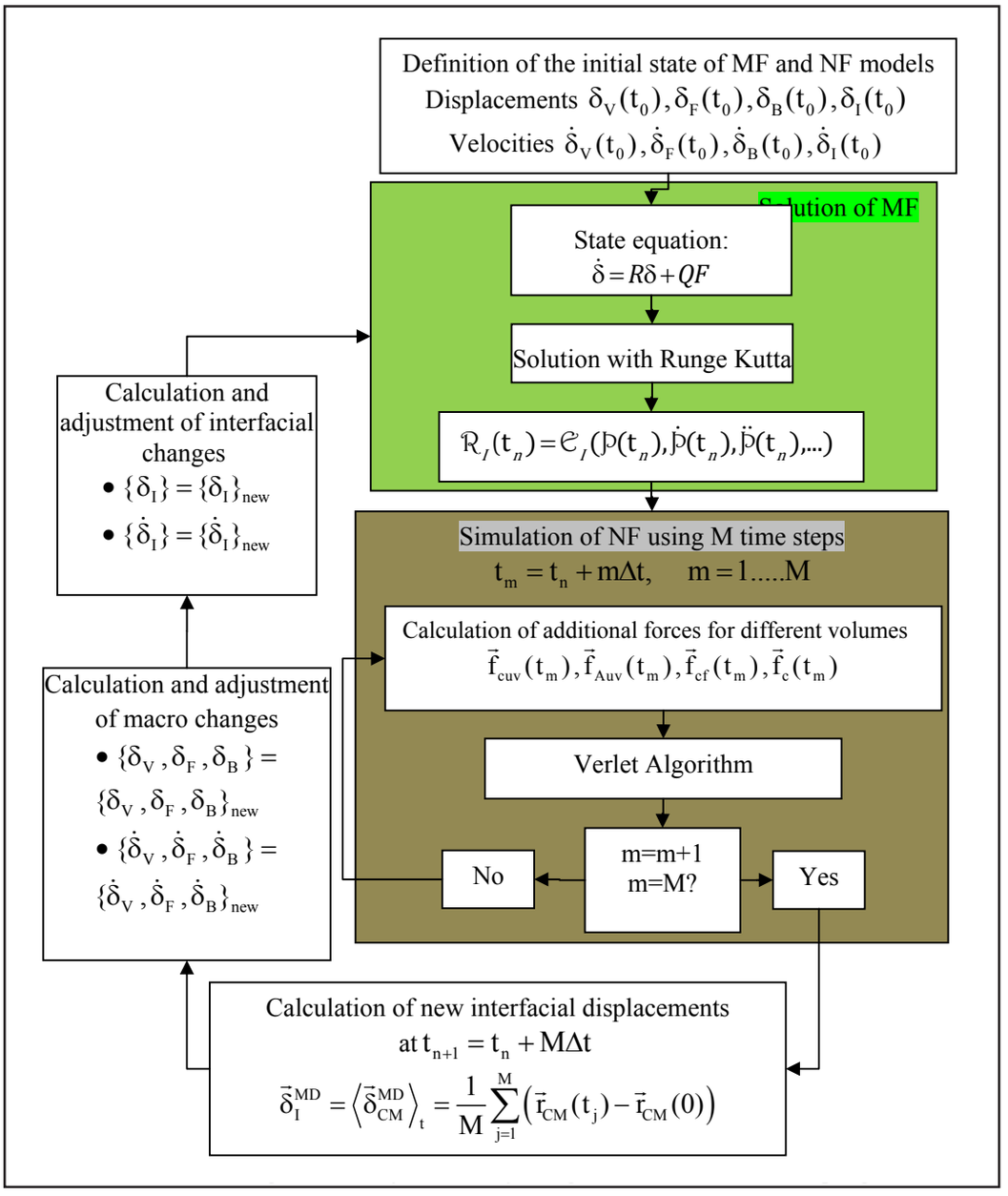
In any case, whether the problem pertains to the subject of solids or fluid dynamics, the general dynamic displacement vector could be expressed as follows:

$$\mathfrak{p}(t)=\mathfrak{u}(t)+\mathfrak{g}(t) \tag{19}$$

where $\mathfrak{g}(t)$ and $\mathfrak{u}(t)$ are the vector of initial degrees of freedom and the elastic vector of the whole system, respectively. By substituting the general dynamic displacement vector in the equation of motion, and using the principle of superposition, we have:

$$\mathcal{C}(\mathfrak{u}(t_n),\dot{\mathfrak{u}}(t_n),\ddot{\mathfrak{u}}(t_n),...)=-\mathcal{C}(\mathfrak{g}(t_n),\dot{\mathfrak{g}}(t_n),\ddot{\mathfrak{g}}(t_n),...) \tag{20}$$

And thus, the initial value problem is converted into the external force problem. If the effects of orders higher than the second derivative of the degrees of freedom are disregarded, and the effects of the



Figue 5: *Dynamic analysis algorithm of MF and NF coupling*

considered orders are assumed as linear (like many common methods, including the finite element), then the equations can be rewritten as follows:

$$\mathcal{C}_K(u(t_n))+\mathcal{C}_D(\dot{u}(t_n))+\mathcal{C}_A(\ddot{u}(t_n))= \quad (\quad(t\quad)) \tag{21}$$
$$-\mathcal{C}_K(g(t_n))-\mathcal{C}_D(\dot{g}(t_n))-\mathcal{C}_A(\ddot{g}(t_n))$$

By arranging the total displacement vector, the state form of the equations can be expressed as:

$$\left(\frac{d}{dt}\right)\vec{Q}=\begin{bmatrix}0 & I\\ -\mathcal{C}_A^{-1}\mathcal{C}_K & -\mathcal{C}_A^{-1}\mathcal{C}_D\end{bmatrix}\vec{Q}+\begin{bmatrix}\mathcal{C}\end{bmatrix} \tag{22}$$
$$-\begin{bmatrix}0\\ \mathcal{C}_A^{-1}\end{bmatrix}\left(\mathcal{C}_K(g(t_n))+\mathcal{C}_D(\dot{g}(t_n))+\mathcal{C}_A(\ddot{g}(t_n))\right)$$

in which, $\vec{Q} = \{u_V, u_F, u_B, u_I, \dot{u}_V, \dot{u}_F, \dot{u}_B, \dot{u}_I\}^T$ is the state vector and the C_K, C_D, and C_A matrices are the resolved zero to second order terms of the general equation of motion.

The solution of unknown elastic displacements within the MF region, i.e. $\{u_V, u_F, u_B, u_I\}$, can be obtained by solving the above state equation and by applying the initial condition IC=0 in the first step, and applying the condition IC=IC_i in the ith step of the macro solution. Then, the interfacial forces are obtained through the following relations:

$$R_I(t_n) = C_I(p(t_n), \dot{p}(t_n), \ddot{p}(t_n), ...) \quad (23)$$

The dynamics of the atom i with mass $m^{(i)}$, at the position $r^{(i)}$, and in the NF regions are described through the Newton's equations of motion. Thus, for different regions belonging to the general NF we have:

$$m_i \ddot{\vec{r}}_i = \vec{f}_i + f_i^D \quad \text{In the inner NF region} \quad (24a)$$

$$m_i \ddot{\vec{r}}_i = \vec{f}_i + \frac{\vec{R}_I^k}{N_I^k} + f_i^D, \quad (\vec{r}_i, \dot{\vec{r}}_i)\Big|_{\text{first step}} = (\vec{p}_{\Gamma(i)}, \dot{\vec{p}}_{\Gamma(i)})\Big|_{\text{it's last step}}$$

Interfacial NF (for the kth IV) (24b)

$$m_i \ddot{\vec{r}}_i = \vec{f}_i + \frac{\vec{f}_{cuv}^k}{N_{UV}^k} + \frac{\vec{f}_{Auv}^k}{N_{UV}^k} + f_i^D \quad (24c)$$

In the surface NF region (for the kth UV)

$$m_i \ddot{\vec{r}}_i = f_i + \frac{\vec{f}_{cf}^k}{N_{FB}^k} + f_i^D \quad (24d)$$

In the free NF region (for the kth FB)

$$m_i \ddot{\vec{r}}_i = f_i + \frac{\sum_{i=1}^{Atom_{RC}} \left(\vec{f}_c^k\right)_i}{N_{CB}^k} + f_i^D \quad (24e)$$

In the common NF region (for the kth CB)

The atoms in the inner NF region only experience the atomic force $\vec{f}_i = \sum_j \vec{f}_{ij}$ and the frictional forces of f_i^D, which result from their neighboring atoms. The atoms existing in the interfacial NF region (which belong to the kth IV) also experience an additional force $(\vec{R}_I^k)$ which is distributed among N_I^k atoms. In addition, the continuity of the fields of the zero- and first-order degrees of freedom should be guaranteed in it. The atoms existing in the surface NF region (which belong to the kth UV) also experience an opposing force $(\vec{f}_{cuv}^k)$ which is distributed among N_S^k atoms. Moreover, they tolerate the force of $\vec{f}_{Auv}^k$ due to the crushing of the system, which itself should be divided by N_S^k atoms.

In the common boundaries of the NF region, some magnitude of force, which arises from the forces of atoms inside the cut-off radius of the contact surface of two NF fields, should be considered. It should be mentioned that, except in the areas of direct contact between surfaces (where the effect of friction is modeled with the inclusion of some impacts), in the above equations, the viscous friction force f_i^D is uniformly applied to the atoms inside the IVs and UVs. Throughout the integration of the above equations for a period of $\Delta t_M = M\Delta t$ (where M is the number of time steps and Δt is the time step duration), the new average displacements are determined by equation (1). The new atomic displacements for the next MF step at time $t_{n+1} = t_n + \Delta t_M$ are again applied in equations (6) and (7a) for the calculation of forces in the next iteration step. The complete algorithm for the simulation of coupling has been given in Figure 5.

In the following sections, three examples of systems in solid mechanics, which could be considered as candidates for using the proposed method, are presented. The first example (as a sample of a closed system) investigates the penny shaped cracks. The second example (as a sample of a semi-open system), follows up on the effects of macro dynamics on the crack nucleation and propagation. Also, the third example demonstrates a not-so-complete arrangement of the probe tip in a Scanning Probe Microscope (SPM).

5. EXAMPLES AND DISCUSSIONS

5.1. Penny shaped cracks (closed system)

Generally, the propagation or even nucleation of many cracks is due to certain structures and behaviors

in nanoscale and smaller. Dislocations inherently exist in many solid state systems, and in some cases, they emerge as a result of certain reactions. They can grow and take a shape similar to a penny. Basically, the model of a penny shaped crack can be obtained by eliminating one or several particles in atomic models. Here, by using the presented approach, a closed system has been considered, in which a nano field is surrounded by the nodes of a macro field. Then several particles are eliminated from the nano field, so that the behavior of the macro and nano fields could be investigated due to the formation of crack. One of the significant applications of this example is the recognition of the complete behavior of a closed system as a result of changes occurring in the nano environment; it can lead to the prediction of events in the nano environment by using the observations of the macro parts.

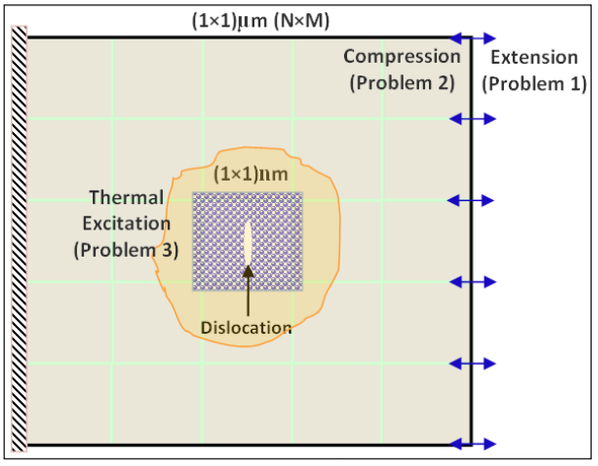


Figure 6: *The penny shape crack (nano field is enlarged)*

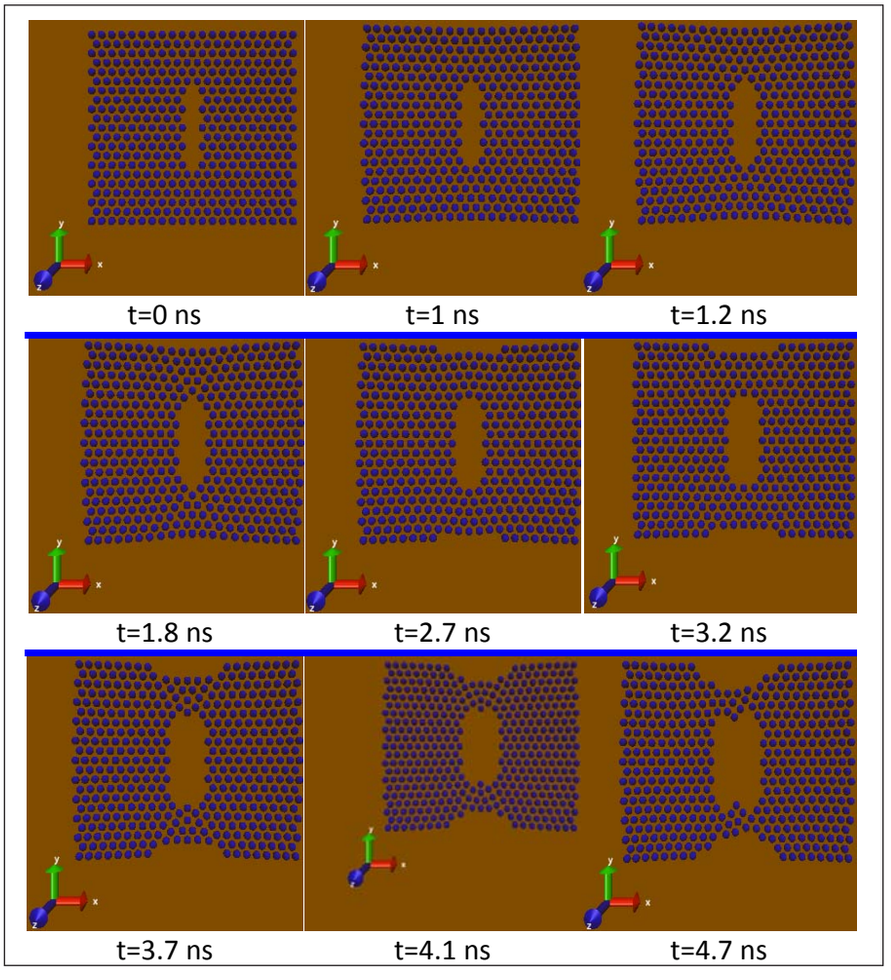


Figure 7: *Effect of applying tensile load on the penny shaped crack*

As it has been depicted in Figure 6, the considered system consists of an aluminum plate with dimensions of 1μ×1μ which is clamped at left end, and a square-shaped part of its midsection (1nm1×nm) is considered as a nano environment. An elliptical crack with the large diameter about 0.4 nm and the small diameter of 0.05 nm has been considered in the center of the nano environment.

First, consider the extension problem due to a tension force. A force large enough is applied to the free end of the cantilever to deform the NF part. Deformations of the NF along the time have been shown in Figure 7. As can be observed, in a relatively long time, a series of initial deformations occurs in the NF. After the elapse of certain time, the deformations are considerably enlarged. Upon the yield point of the NF, deformations grow more and more.

Now, consider the problem of compression of the free end of the cantilever. A force large enough is applied to the free end of the cantilever to deform the NF. Deformations of the NF region have been illustrated in Figure 8. The behavior of this system is very similar to the previous case (although, in the reverse direction); with the difference that the processes take longer time because of the higher resistance of the system to compression. As the figure shows, in a relatively long time, a series of initial deformations occur in the NF.

With a finer sketch, the small reshaping of plate may be observed. Figure 9 shows the finer sketch by enlarging the size of atoms in view for some snapshots of Figure 8. It can be observed that the area of hole is decreasing along the time and it moved to right and finally exits from the end right.

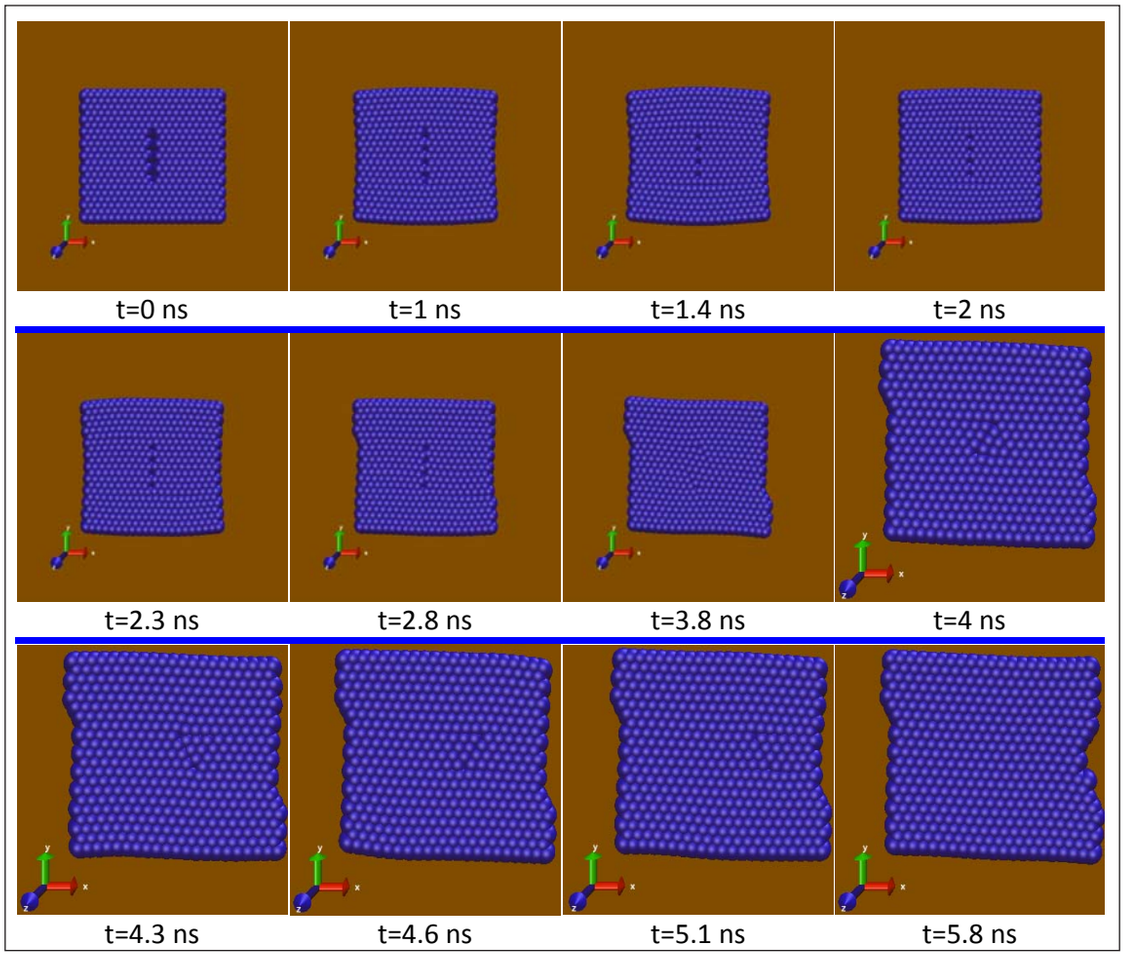


Figure 8: *Effect of applying compressive load on the penny shaped crack*

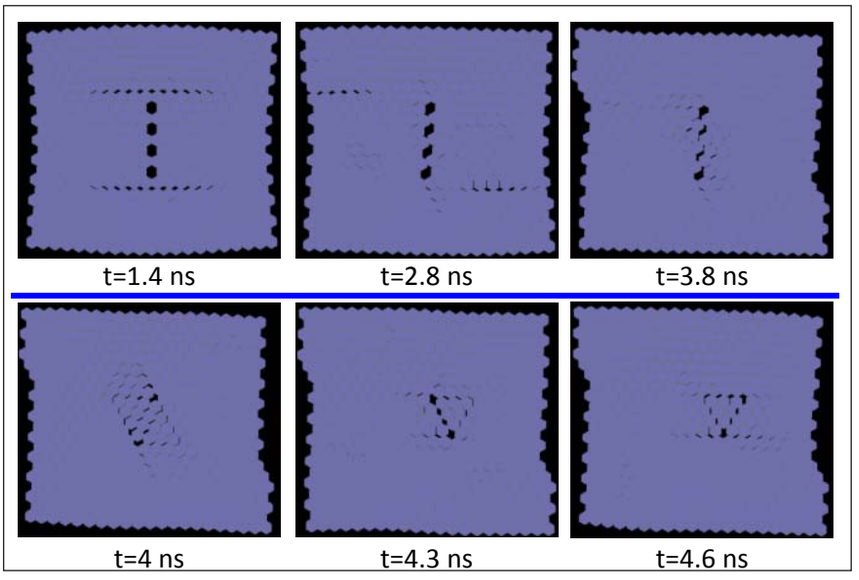


Figure 9: *The fine sketch of deformation in compression test*

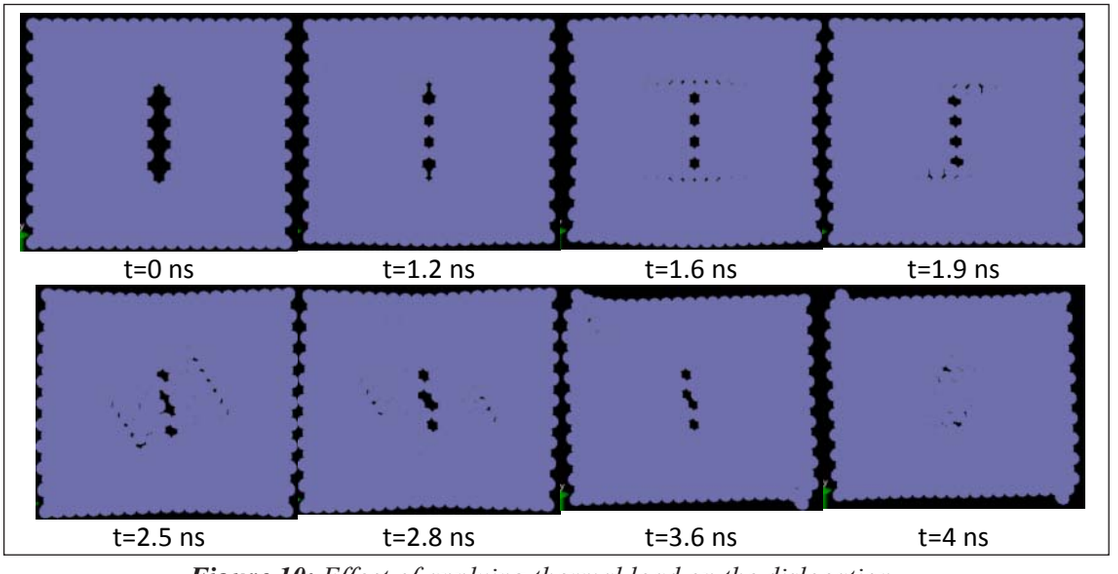


Figure 10: *Effect of applying thermal load on the dislocation*

This is due to the stiffness of macro scale model at the end left.

The third problem involves the behavior of the system due to the environment's temperature increasing. By using the classical NVT algorithm, system's temperature has been increased. It has been observed that by applying the relatively large amounts of heat, the crack area is reduced, but not eliminated. However, it leans to move along the right direction.

5.2. Macro dynamics effect on the propagation of cracks (semi-open system)

Despite the fact that in many cases, the nucleation and propagation of a crack begins within an object, there are also many cases in which the nucleation and propagation of crack is caused by a macro force. To show the capability and effectiveness of the suggested method for semi-open problems, the process of nucleation and propagation of cracks due

to an external load on the edge of a slotted plate is analyzed.

The considered system consists of an aluminum plate with dimensions of 1μ×1μ which is clamped at left end, and a square-shaped part of its midsection (1nm1×nm) is considered as a nano environment. The slot in the Figure 11 clearly shows the positions of the macro and nano fields.

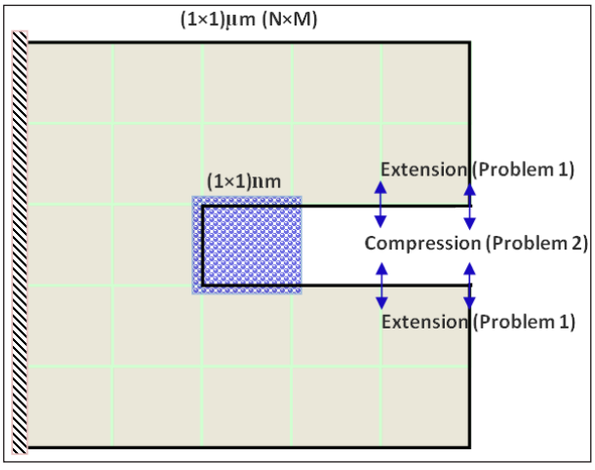


Figure 11: *Macro and nano fields in the case of nucleation and propagation of crack caused by the application of mechanical load*

First, we examine the application of tensile load on the edges of the macro slot. The deformation of NF has been illustrated in Figure 12. As it is shown, the NF system resists for a long time against the application of the load, but it eventually yields to the load and deforms considerably. When compressive load is applied and the edges have been closed to each other in the MF environment, although absolute yield doesn't happen, but very small and localized dislocations are observed in the form of a relatively harmonic wave.

5.3. Dynamic movement of a nano object on the tip of a cantilever probe (open system)

In many cases (like in cell manipulation or imaging processes), it is necessary to use a relatively large surface to displace the environment which hold the cell from one location to another. Here, it is assumed that, instead of a cell, we want to investigate the behavior of a very small solid metal object as a result of the movement of its base, by using a metal plate in larger dimensions. Assume a rectangular shape plate (like the two-dimensional case of a cantilever, or an approximation of the configuration of an AFM probe tip), with the dimensions given in the Figure 14.

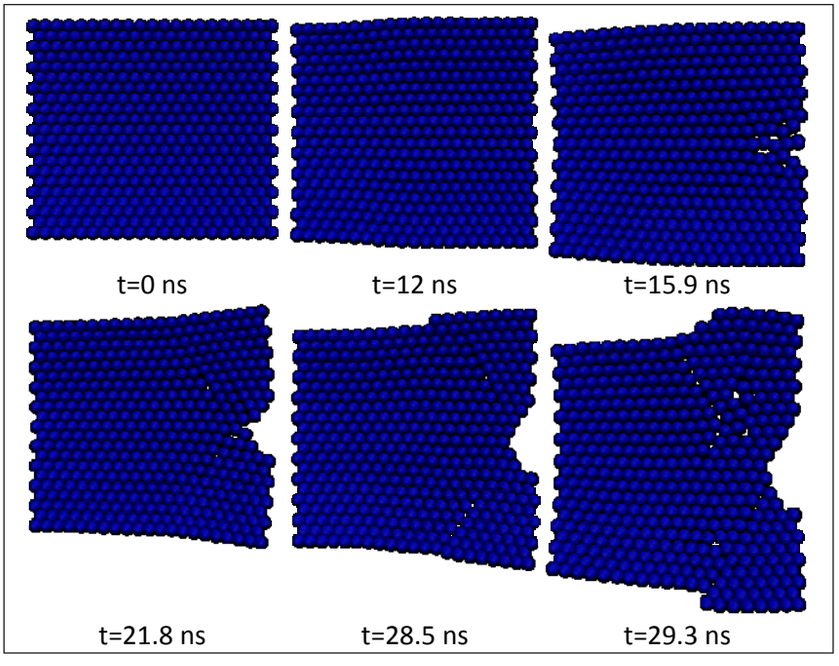


Figure 12: *Nano field in the case of nucleation and propagation of crack due to the application of macro-mechanical load; tension problem*

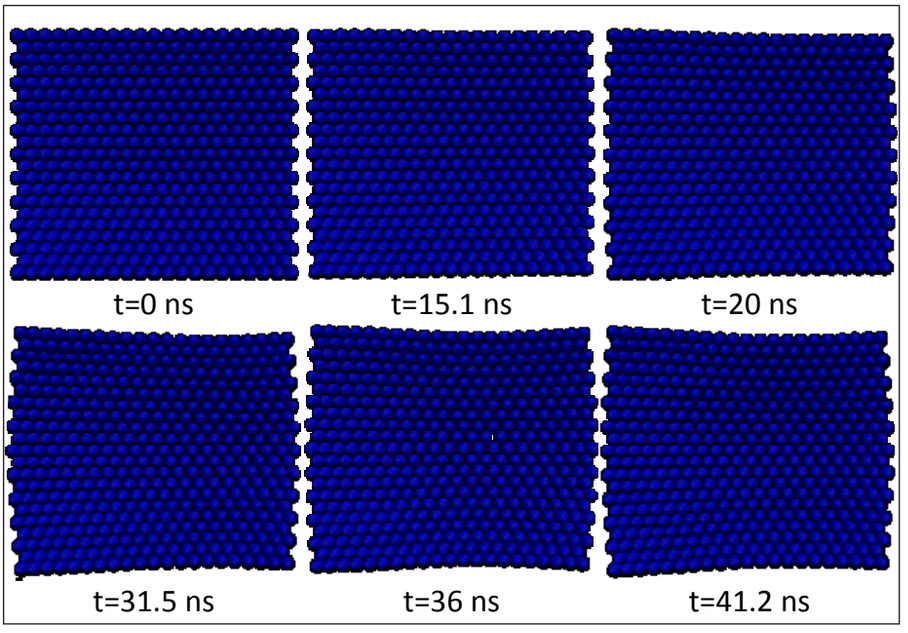


Figure 13: *Nano field in the case of nucleation and propagation of crack due to the application of macro-mechanical load; compression problem*

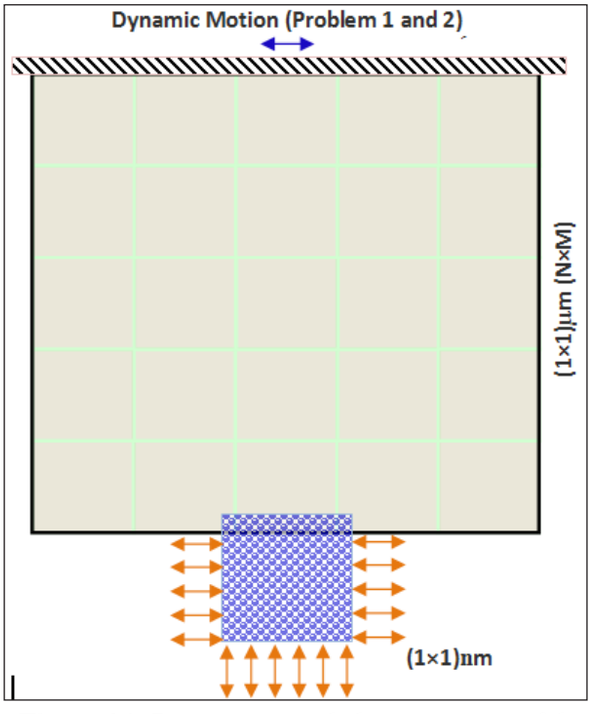


Figure 14: *Dimensions and characteristics of the coupled system*

We consider a system in nano dimensions and with the properties of silicone as a body (particle) attached to this cantilever. The cantilever is fixed at the top, and its base is moved with a constant velocity. As Figure 15 shows, the movement of this system is very similar to the movement of a rigid body. Considering the assumption that both fields are metallic, this conclusion seems reasonable. Of course, to demonstrate the existence of considerable force in the interface of the two fields, the R_I forces have been shown in horizontal and vertical directions, in Figure 16.

Now assume that a nano object, but with bioorganic characteristics (which are often viscoelastic properties), is located on the cantilever beam. For a more reasonable effect of the macro environment on the nano environment, the macro-cantilever is also assumed to be made of a more flexible material. As Figure 17 shows, a flexible deformation will occur in the nano field.

In Figure 18, the diagram of the normalized average displacement of NF particles together with the normalized displacement of the node adjacent to NF has been plotted in the MF environment. It is obvious that the movement of NF is in the vicinity of the node adjacent to MF, and it only has small oscillatory motions around it.

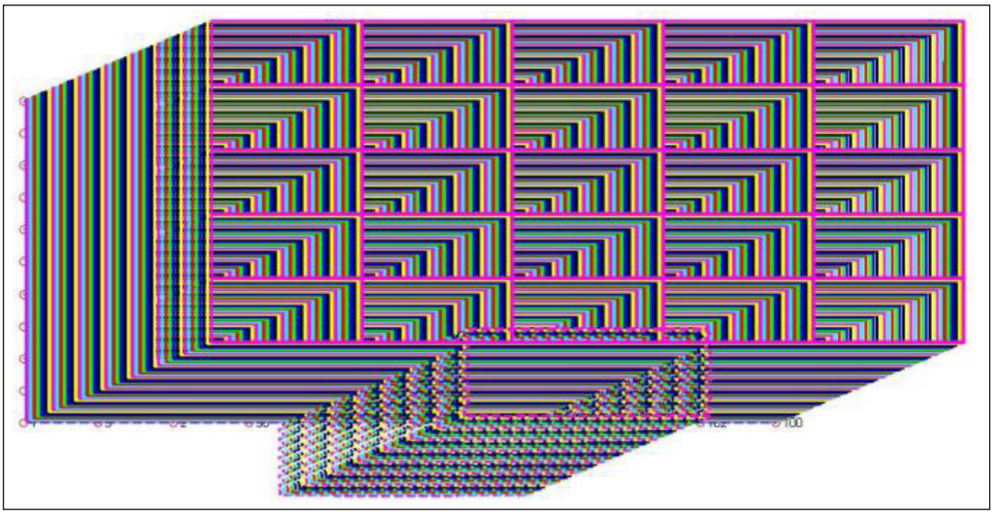


Figure 15: *Displacement of the MF and NF fields due to the displacement of the MF base in the x-y plane; movement of a hard system*

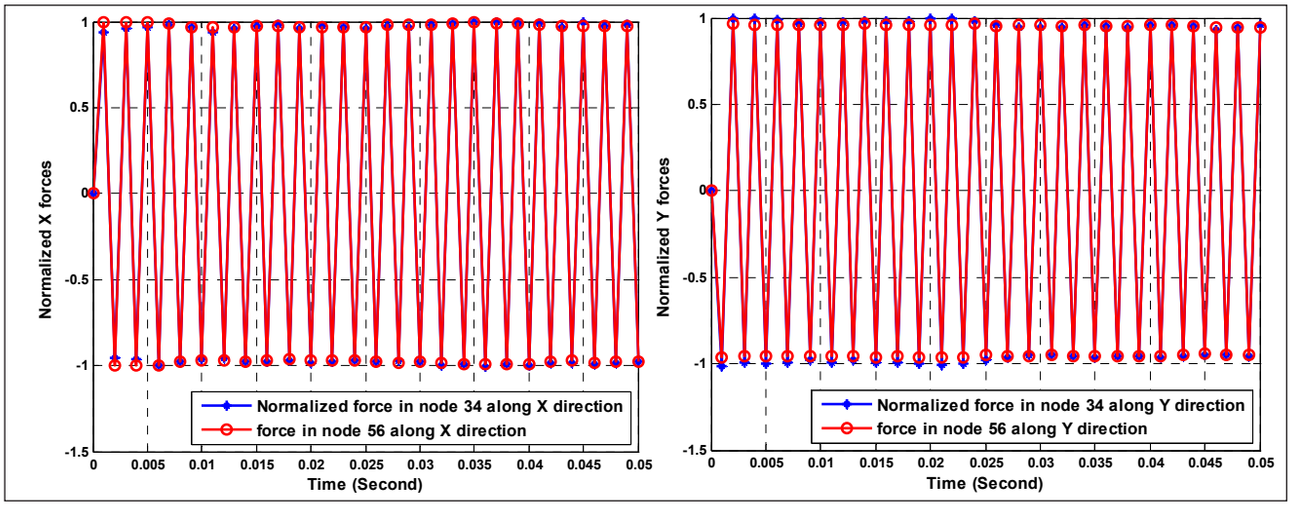


Figure 16: *Interfacial forces (R_I) in horizontal and perpendicular directions for the movement of a metallic nano field on a metallic macro field*

6. CONCLUSION

A method has been presented for the coupling of the continuum and atomic scales together. In the present model, the undesirable effects of free surfaces, common surfaces, and surfaces close to the interface with the macro field have been removed, and after offering a practical and notable procedure for the dynamics of systems in general, seven problems (in the form of three examples) have been presented to showcase the practicality, simplicity, and the effectiveness of this method.

To generalize the issue, the macro/nano-related problems were divided into two groups of closed and open systems. Then, the damped dynamics of these systems in general cases were presented. Also, by using the presented approach, several examples of the closed, open, and semi-open cases were solved. The crack nucleation and propagation due to the macro dislocation (a penny shaped crack) was explored. The most important outcome of this example is the considerable influence of dislocation on the propagation of crack.

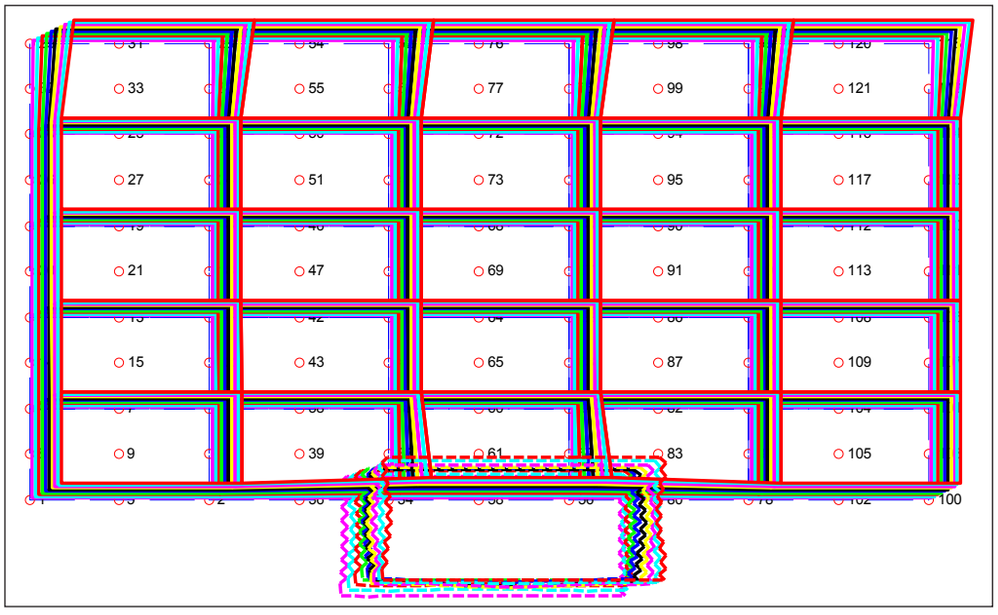


Figure 17: *Displacement of the MF and NF fields due to the displacement of the MF base in the x-y plane; movement of a soft system*

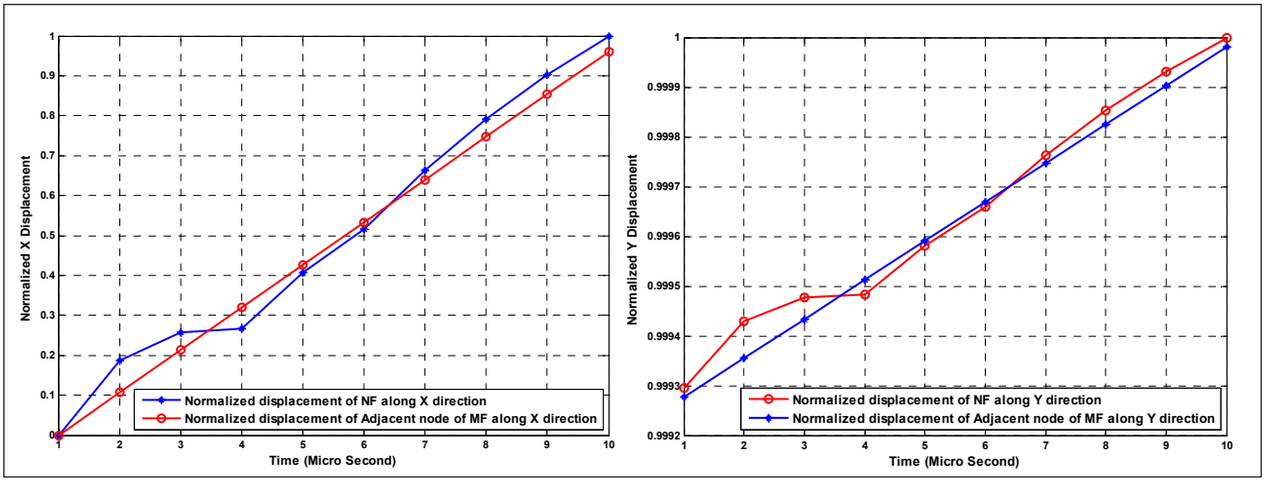


Figure 18: *Displacement of the MF and NF fields due to the displacement of the MF base in the x and y directions*

As a case for a semi-open system, the process of nucleation and propagation of cracks due to the application of an external load on the edge of a slotted plate was presented. In the problem dealing with the application of tensile load on the edges of the macro slot, the NF system resists for a long time against the application of the load, but it eventually yields to the load and undergoes deformation. In addition, as a case of open system, two metallic and bioorganic nanorobotic systems were considered via the attachment of an object (particle) to the cantilever probe. Rigidity of the first case and the considerable flexibility of the second case were demonstrated. With respect to the obtained results, it was demonstrated that the presented method can be applied for the simulation of systems with considerable dimensions, and for relatively large time ranges. The use of coarse-grained molecular dynamics (CGMD) in this method has made this capability possible. Also, the use of finite element

method, and the presentation of an element which is capable of being applied for the electromechanical systems, has greatly expanded the range of application of this method.

7. ACKNOWLEDGMENT

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