

Atomic-scale finite element method in multiscale computation with applications to carbon nanotubes

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We have developed an accurate atomic-scale finite element method (AFEM) that has exactly the same formal structure as continuum finite element methods, and therefore can seamlessly be combined with them in multiscale computations. The AFEM uses both first and second derivatives of system energy in the energy minimization computation. It is faster than the standard conjugate gradient method which uses only the first order derivative of system energy, and can thus significantly save computation time especially in studying large scale problems. Woven nanostructures of carbon nanotubes are proposed and studied via this new method, and strong defect insensitivity in such nanostructures is revealed. The AFEM is also readily applicable for solving many physics related optimization problems.

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I. INTRODUCTION

The fastest computer in the world today can handle up to a billion atoms,^{1,2} which correspond only to a small cube of 1 μm in size. This size may increase to 10 μm in 15 years, since computer power doubles every 18 months based on Moore's law.³ Even with fast increase in computer power, the computational limit of atomistic simulations is still far short to predict the macroscale properties of materials directly from nano and microstructures. In this letter, we propose a new computational method that significantly increases the current computational limit from two aspects. First, we develop an accurate atomic scale finite element method (AFEM) for stable atomic structures (e.g., carbon nanotube) and well-defined interatomic potentials.⁴ The AFEM is faster than the widely used conjugate gradient method because it uses both first and second order derivatives of system energy. Second, different from other atomistic methods (e.g., conjugate gradient method, molecular dynamics), the proposed AFEM has exactly the same formal structure as continuum finite element methods (FEM). The combined AFEM/FEM provides a seamless multiscale simulation method that significantly reduces the degree of freedom and therefore enables computation at a much larger scale (possibly macroscale).

The conventional continuum approach such as FEM is successful for micro- and macroscale problems, but cannot describe the behavior of discrete atoms involving multibody interactions. On the other hand, atomistic simulations have been used to gain fundamental understanding of material behavior at the nanoscale, but they are difficult to scale up due to a large number of degrees of freedom involved. Multiscale computational methods⁵⁻¹¹ have emerged as a viable means to study materials and systems across different scales. The basic idea is to use atomistic simulation methods for domains governed by nanoscale physics laws and use continuum

FEM for the rest in order to reduce degrees of freedom. Existing multiscale computational methods involve artificially introduced interfaces between domains of different simulation methods (e.g., conjugate gradient method or molecular dynamics for atomistic domains and FEM for continuum domains). These interfaces may lead to computation errors (e.g., spurious or "ghost" force⁶) and add significant computational effort to ensure interface conditions between atomistic and continuum models. Success of multiscale computation requires the development of a unified simulation method that is based on the same theoretical framework for both atomistic (discrete) and continuum analyses. Since continuum FEM is very mature and successful, we develop an atomic-scale finite element method (AFEM) that uses atoms as FEM nodes in the atomistic analysis. It accurately captures the discreteness and multibody interactions of atoms, and has exactly the same formal structure as continuum FEM such that the combined AFEM and continuum FEM avoid artificial interfaces. Furthermore, AFEM is as accurate as molecular mechanics, but is faster than the latter because it uses both first and second order derivatives of energy.

II. ATOMIC-SCALE FINITE ELEMENT METHOD

The equilibrium configuration of atoms corresponds to a state of minimal energy. For a system of N atoms, the total energy in the system is $E_{\text{tot}}(\mathbf{x})$, where $\mathbf{x}=(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)^T$, \mathbf{x}_i is the position of atom i , and E_{tot} is evaluated from the interatomic potential. The state of minimal energy corresponds to

$$\frac{\partial E_{\text{tot}}}{\partial \mathbf{x}} = 0. \quad (1)$$

The Taylor expansion of E_{tot} around an initial guess $\mathbf{x}^{(0)}=(\mathbf{x}_1^{(0)}, \mathbf{x}_2^{(0)}, \dots, \mathbf{x}_N^{(0)})^T$ of the equilibrium state gives

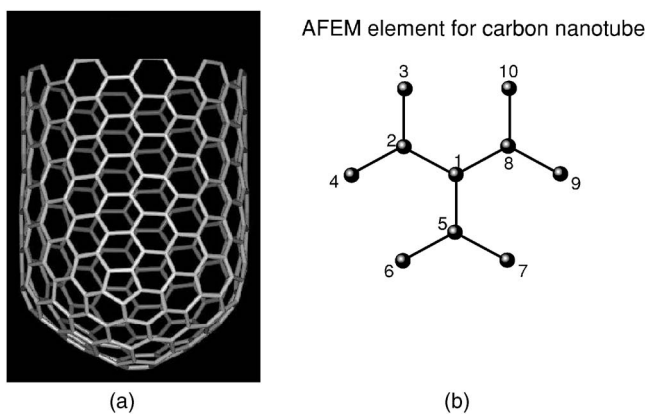


FIG. 1. (a) Schematic diagram of a single wall carbon nanotube; (b) an atomic-scale finite element for carbon nanotubes.

$$E_{\text{tot}}(\mathbf{x}) \approx E_{\text{tot}}(\mathbf{x}^{(0)}) + \left. \frac{\partial E_{\text{tot}}}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}^{(0)}} \cdot (\mathbf{x} - \mathbf{x}^{(0)}) + \frac{1}{2} (\mathbf{x} - \mathbf{x}^{(0)})^T \cdot \left. \frac{\partial^2 E_{\text{tot}}}{\partial \mathbf{x} \partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}^{(0)}} \cdot (\mathbf{x} - \mathbf{x}^{(0)}). \quad (2)$$

Its substitution into Eq. (1) yields the following governing equation for the displacement $\mathbf{u} = \mathbf{x} - \mathbf{x}^{(0)}$:

$$\mathbf{K}\mathbf{u} = \mathbf{P}, \quad (3)$$

where $\mathbf{K} = \partial^2 E_{\text{tot}} / \partial \mathbf{x} \partial \mathbf{x} |_{\mathbf{x}=\mathbf{x}^{(0)}}$, and $\mathbf{P} = -\partial E_{\text{tot}} / \partial \mathbf{x} |_{\mathbf{x}=\mathbf{x}^{(0)}}$ which represents the steepest descent direction of E_{tot} . The above equation is identical to the governing equation in continuum FEM if atoms are replaced by FEM nodes. In fact, \mathbf{K} and \mathbf{P} are called the stiffness matrix and nonequilibrium force vector, respectively, in FEM. For a nonlinear system, Eq. (3) is solved iteratively until \mathbf{P} reaches zero, $\mathbf{P} = 0$. The iteration involves the following steps:

- (i) Evaluate \mathbf{K} and \mathbf{P} at $\mathbf{x} = \mathbf{x}^{(0)}$;
- (ii) Solve $\mathbf{u} = \mathbf{x} - \mathbf{x}^{(0)}$ from Eq. (3);
- (iii) Update $\mathbf{x}^{(0)}$ by $\mathbf{x}^{(0)} + \mathbf{u}$.

The above steps are repeated until $\mathbf{P} = 0$.

Since each atom interacts only with finite neighbor atoms (but not necessarily nearest-neighbor atoms), the first and second order derivatives, $\partial E_{\text{tot}} / \partial \mathbf{x}_i$ and $\partial^2 E_{\text{tot}} / \partial \mathbf{x}_i \partial \mathbf{x}_j$, of E_{tot} with respect to atom i can be calculated via a small subset of atoms including atom i and its neighbor atoms. Such a subset of atoms is called an element in AFEM, and the composition of element depends on the atomic structure and nature of atomistic interactions, as to be discussed in the example shown in Fig. 1. The contribution from this element to \mathbf{K} is called the element stiffness matrix $\mathbf{K}_i^{\text{element}}$ such that \mathbf{K} is the assemble of all element stiffness matrices.

We use a carbon nanotube (CNT) shown in Fig. 1 as an example to illustrate the AFEM element. Figure 1 shows a three-dimensional AFEM element for CNT containing a central atom (No. 1), three nearest-neighbor (No. 2,5,8) and six second-nearest-neighbor atoms (Nos 3,4,6,7,9, and 10). The atomistic interaction among carbon atoms is characterized by multibody interatomic potentials (e.g., Refs. 12–14) which indicate that each atom (No. 1) on a CNT interacts with not

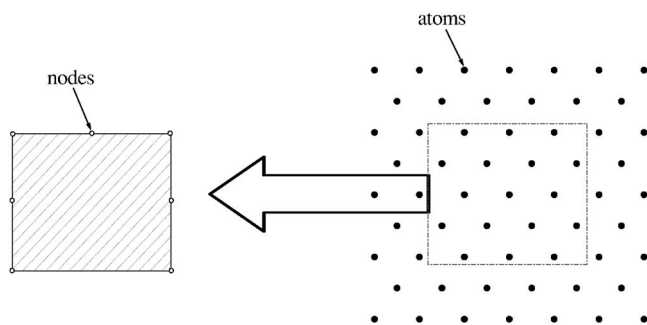


FIG. 2. Schematic diagram of continuum finite element vs discrete atoms.

only three nearest-neighbor atoms but also six second-nearest-neighbor atoms via the bond angle change. For example, energy stored in an atomic bond between atoms 1 and 2 depends on not only the bond length but also angles with neighbor bonds 1–5, 1–8, 2–3, and 2–4, reflecting the multi-body nature of atomistic interactions. Therefore, the position change of central atom 1 influences energy stored in nine atomic bonds within this element shown in Fig. 1. Such an element captures interactions between the central atom and all neighbor atoms, and is used to calculate $(\partial E_{\text{tot}} / \partial \mathbf{x}_1)$ and $(\partial^2 E_{\text{tot}} / \partial \mathbf{x}_1 \partial \mathbf{x}_j)$ associated with the central atom. It gives the following element stiffness matrix $\mathbf{K}^{\text{element}}$ and nonequilibrium force vector $\mathbf{P}^{\text{element}}$:

$$\mathbf{K}^{\text{element}} = \begin{bmatrix} \left(\frac{\partial^2 E_{\text{tot}}}{\partial \mathbf{x}_1 \partial \mathbf{x}_1} \right)_{3 \times 3} & \left(\frac{1}{2} \frac{\partial^2 E_{\text{tot}}}{\partial \mathbf{x}_1 \partial \mathbf{x}_j} \right)_{3 \times 27} \\ \left(\frac{1}{2} \frac{\partial^2 E_{\text{tot}}}{\partial \mathbf{x}_j \partial \mathbf{x}_1} \right)_{27 \times 3} & (\mathbf{0})_{27 \times 27} \end{bmatrix}, \quad (4)$$

$$\mathbf{P}^{\text{element}} = \begin{bmatrix} -\left(\frac{\partial E_{\text{tot}}}{\partial \mathbf{x}_1} \right)_{3 \times 1} \\ (\mathbf{0})_{27 \times 1} \end{bmatrix}. \quad (5)$$

Therefore, each row in the stiffness matrix \mathbf{K} assembled from element stiffness matrices has at most 30 nonzero components (since each element has tens atoms) such that \mathbf{K} is sparse and the number of nonzero components is on the order N , i.e., $O(N)$, where N is the total number of atoms in the system. It is important to point out that AFEM does not involve any approximations of continuum FEM (e.g., interpolation), and gives accurate results.

Even though AFEM and continuum FEM have exactly the same formal structures, they are different in many aspects besides the important difference in discreteness. First, energy is partitioned into elements in continuum FEM, and energy in each element is evaluated in terms of nodes within the element. Such an element cannot capture the multi-body atomistic interactions since it does not have access to atoms beyond the element. For example, Fig. 2(a) shows a conventional eight-node continuum finite element used to represent atoms within the same area of the element shown in Fig. 2(b). Energy given by continuum FEM depends only on these eight nodes, but energy associated with atoms inside the element depends on atoms outside due to multibody ato-

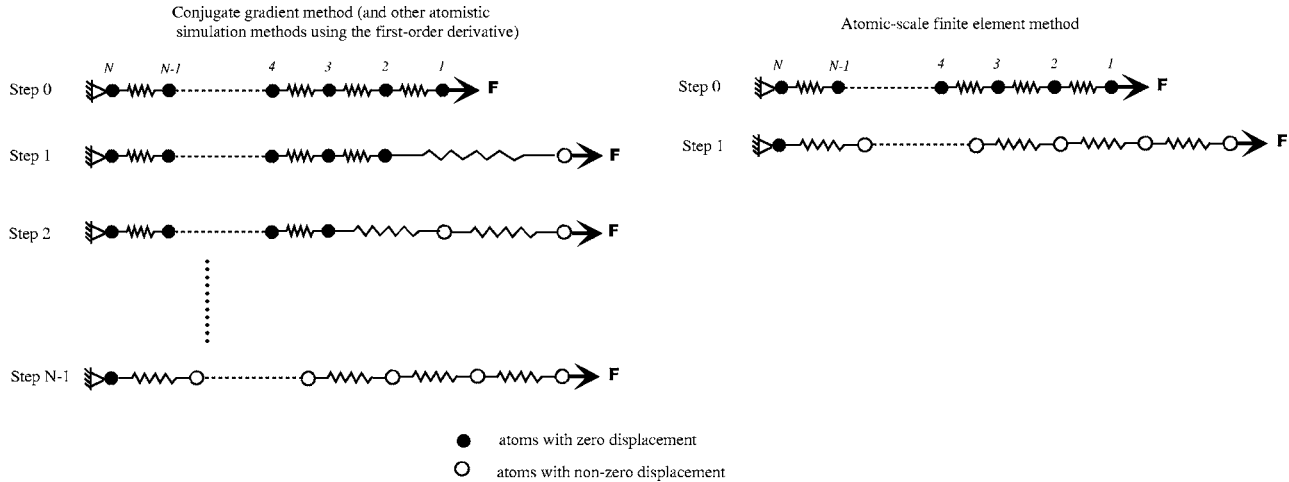


FIG. 3. Schematic diagram to illustrate the difference between conjugate gradient method and atomic-scale finite element method for a linear, one-dimensional atomic chain.

mistic interactions. In AFEM, on the contrary, energy is not partitioned into elements. Instead, only the first and second order derivatives of E_{tot} are evaluated directly from the AFEM element. The AFEM elements overlap in space in order to account for multibody atomistic interactions. Another difference between AFEM and continuum FEM is that AFEM is material specific, while continuum FEM is generic for all materials. An AFEM element depends on the atomic structure and interatomic potential. For example, an AFEM element for diamond contains 17 atoms, including four nearest-neighbor atoms and 12 second-nearest-neighbor atoms. Last, the element stiffness matrix in Eq. (4) looks very different from its counterpart in continuum FEM because the AFEM element focuses on the central atom (No. 1).

III. COMPUTATIONAL SPEED OF AFEM

The computation in AFEM (as well as in continuum FEM) consists of three parts,

- (i) computation of the stiffness matrix \mathbf{K} and nonequilibrium force vector \mathbf{P} in each iteration step;
- (ii) solving $\mathbf{K}\mathbf{u}=\mathbf{P}$ in each iteration step; and
- (iii) repeat of parts (i) and (ii) for all iteration steps until $\mathbf{P}=\mathbf{0}$, if the system is nonlinear.

For linear systems the Taylor expansion in Eq. (2) becomes exact such that Eq. (3) needs to be solved only once. AFEM is an order- N computational method because (i) the effort to compute \mathbf{K} and \mathbf{P} is $O(N)$; and (ii) the effort to solve $\mathbf{K}\mathbf{u}=\mathbf{P}$ in Eq. (3) is $O(N)$ due to the sparseness of \mathbf{K} .¹⁵ The conjugate gradient method widely used in atomistic studies is an order- N^2 method even for linear systems, i.e., its computational effort increases much more rapidly than the increase of N for a large system. This difference in scaling with N is because AFEM uses both first and second order derivatives of E_{tot} such that any nonzero component in the nonequilibrium force \mathbf{P} immediately leads to nonzero displacement \mathbf{u} in the entire system via the second order derivative \mathbf{K} and Eq. (3), and therefore AFEM reaches energy minimum in one step (for linear systems). The conjugate gradient method

utilizes only the first order derivative, and takes steps that are on the order N to reach the entire system. We use the example of a one-dimensional chain of N atoms subject to a force \mathbf{F} shown in Fig. 3 to further illustrate the difference in computational efforts between the conjugate gradient method and AFEM. For the conjugate gradient method which uses first order derivatives only, one atom moves in each iteration step and it takes $N-1$ steps for the system to reach equilibrium. For AFEM which uses both first and second order derivatives, all atoms move in each iteration step, and only one iteration step is needed for a linear system.

For nonlinear systems, energy minimum is reached iteratively in AFEM. The computational effort in each iteration step is still $O(N)$, but the overall computational effort is $O(M \times N)$, which M is the number of iteration steps which, in general, increases with the system size N , particularly for energy surface displaying rapid changes (e.g., complicated thin valleys and tall mountain passes). The Taylor expansion in Eq. (2) then holds only in very small range (immediate neighborhood of $\mathbf{x}^{(0)}$) such that the iteration steps M may become large and AFEM may not be an order- N method anymore. However, for some problems with stable atomic structures and well-defined interatomic potentials,⁴ the number of iteration steps M to reach energy minimum may be approximately independent of N . Figure 4 shows the number of steps M and deformed configurations for four (5,5) armchair CNTs with 400, 800, 1600, and 3200 atoms calculated from AFEM (not combined with continuum FEM). The CNTs, which are initially straight with two ends fixed, are subject to the same lateral force 50 eV/nm in the middle. The number of steps M varies very little with N , from 43 to 31 and averaged at 35. In fact, the CPU time¹⁶ shown in Fig. 4 indeed displays an approximately linear dependence on N . We have also calculated a 605-nm-long (5,5) CNT with 48 200 atoms. The number of steps M is 35, which is in the same range as those in Fig. 4.¹⁷

For comparison we study the same four (5,5) armchair CNTs with 400, 800, 1600, and 3200 atoms as in Fig. 4 via the conjugate gradient method. The program we use is the UMCGG subroutine in IMSL.¹⁸ Figure 5(a) shows the number

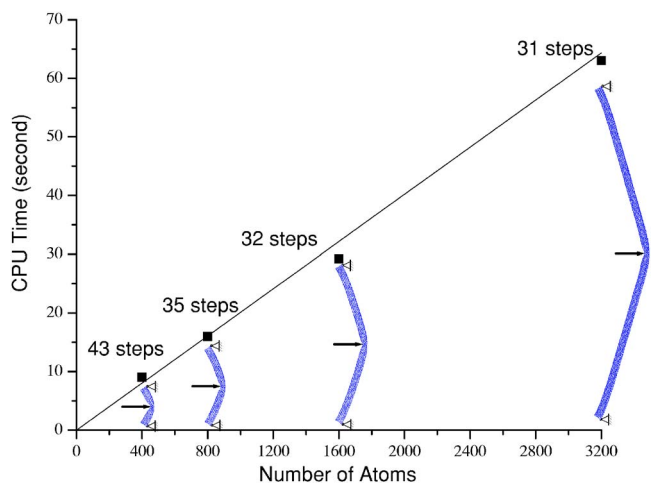


FIG. 4. (Color online) CPU time for atomic-scale finite element method (AFEM) scales linearly with number of atoms for (5,5) carbon nanotubes. The numbers of iteration steps are approximately independent of the number of atoms, which implies that, for carbon nanotubes subject to deformation, the AFEM is an order- N method.

of iteration steps M , which increases with the system size N , and is approximately proportional to N . Since the computational effort within each step is $O(N)$, the overall computational effort is $O(N^2)$ for conjugate gradient method. In fact, Fig. 5(b) shows the CPU time for conjugate gradient method, which is approximately two orders of magnitude larger than that for AFEM shown in Fig. 4. Furthermore, the CPU time scales with the square of number of atoms, i.e., $O(N^2)$, such that the conjugate gradient method is an order- N^2 method.

Even when AFEM loses its order- N characteristics, it is still a very efficient method. This is because any nonzero component of the nonequilibrium force \mathbf{P} immediately leads to nonzero displacement \mathbf{u} in the entire system in each iteration step via the second order derivative \mathbf{K} and Eq. (3) for AFEM. On the contrary, any nonequilibrium force on an atom only affects its neighbor atoms during each iteration in the standard conjugate gradient method since only the first order derivative is used. The number of iteration steps M , in general, depends on many factors such as the system size N , the distance between the initial guess and equilibrium point (minimal energy), and the roughness of energy surface. If the latter two remain essentially unchanged, the number of iteration steps M may not increase with the system size N , as shown in Fig. 4 for carbon nanotubes, such that AFEM is still an order N method.

In order to further explore the order- N nature of AFEM for stable atomic structures and well-defined interatomic potentials,⁴ we show in Fig. 6 the nanoindentation of a plane of atoms. For simplicity, atoms have triangular lattice structure, and are characterized by the Lennard-Jones 6–12 potential. The top surface is subject to the vertical displacement according to a rigid indenter (Fig. 6); the bottom surface is fixed in the vertical direction but allows free sliding in the horizontal direction; and two lateral surfaces are free. We show three sets of atoms, 400 ($=20 \times 20$), 1600 ($=40 \times 40$), and 6400 ($=80 \times 80$), in Fig. 6. The number of iteration steps is $M=38, 38$, and 37 , respectively. Therefore, the number of

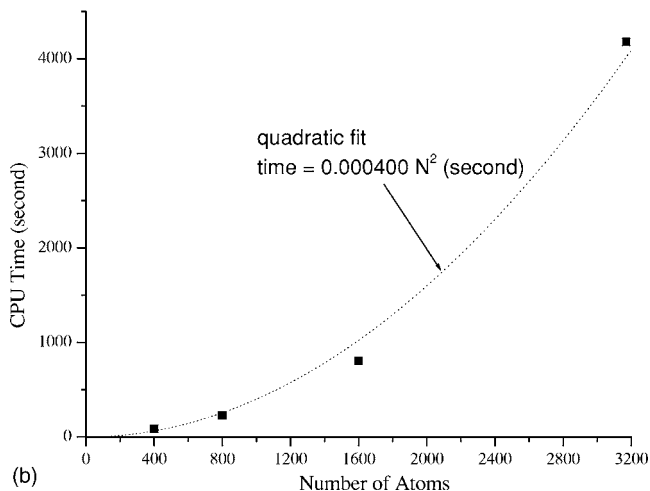
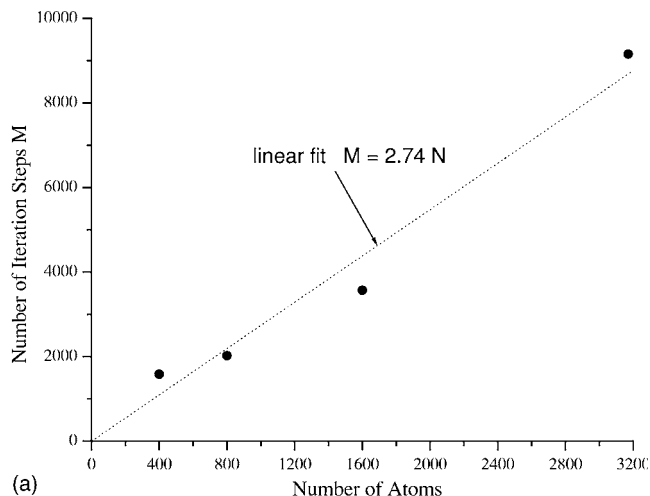


FIG. 5. Number of iteration steps for conjugate gradient method increases linearly with the number of atoms for (5,5) carbon nanotubes, while the CPU time scales with the square of number of atoms. This implies that the conjugate gradient method is an order- N^2 method; (a) number of iteration step; (b) CPU time.

iteration steps is essentially independent of the system size N .

IV. STABILITY AND CONVERGENCE OF AFEM

We study the stability and convergence of AFEM for non-linear interatomic potentials that may display softening behavior. The stability and convergence are ensured if energy in the system decreases in every step, i.e., $\mathbf{u} \cdot \mathbf{P} > 0$, where \mathbf{u} is the displacement increment, and \mathbf{P} is the nonequilibrium force in Eq. (3) and it represents the steepest descent direction of E_{tot} . From Eq. (3), a sufficient condition for $\mathbf{u} \cdot \mathbf{P} > 0$ is that the stiffness matrix \mathbf{K} is positive definite. For problems involving neither material softening nor nonlinear bifurcation, \mathbf{K} is usually positive definite and AFEM is stable, as in the examples shown in Figs. 4 and 6. For nonpositive definite \mathbf{K} , we replace \mathbf{K} by $\mathbf{K}^* = \mathbf{K} + \alpha \mathbf{I}$, where \mathbf{I} is the identity matrix and α is a positive number to ensure the positive definiteness of \mathbf{K}^* which guarantees $\mathbf{u} \cdot \mathbf{P} > 0$. It is important to note that the state of minimal energy is independent of α .

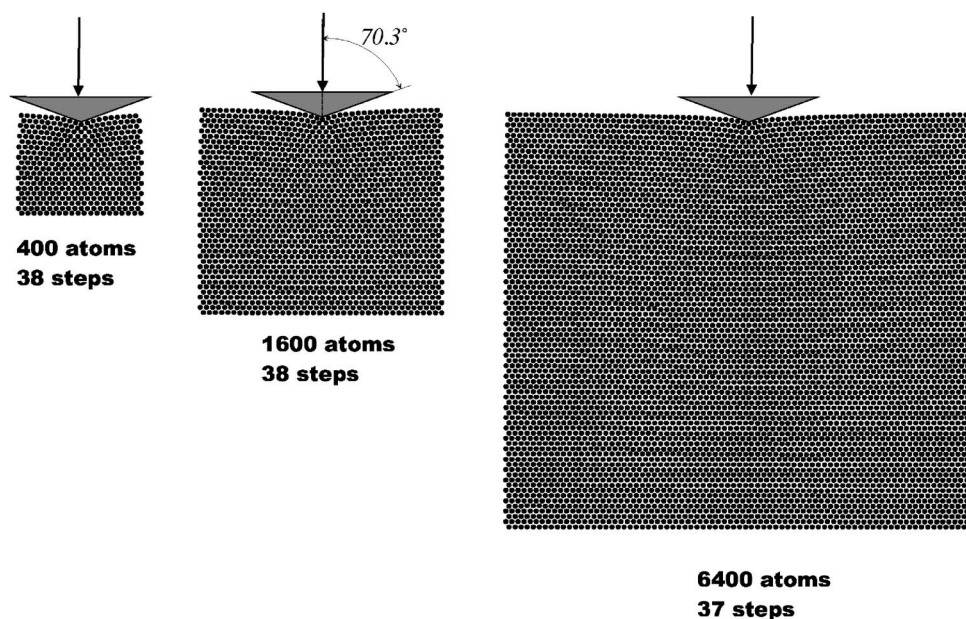


FIG. 6. Number of iteration steps M and deformed configurations of a plane of atoms subject to nanoindentation on the top surface. The half angle of the nanoindenter is 70.3° , and the indentation depth is twice the atomic spacing: (a) 400 atoms; (b) 1600 atoms; (c) 6400 atoms.

This is because the energy minimum is characterized by $\mathbf{P}=\mathbf{0}$, and is independent of \mathbf{K} or \mathbf{K}^* . In fact, at (and near) the state of minimum energy, such modification of \mathbf{K} is unnecessary because the stiffness matrix \mathbf{K} becomes positive definite. We use an example of a (7,7) armchair CNT under compression to examine the stability of AFEM. Figure 7 shows three stages of a 6-nm-long CNT at the compression strain of 0%, 6% (prior to bifurcation), and 7% (post-bifurcation). The stiffness matrix \mathbf{K} experiences nonpositive definiteness between the last two stages, but becomes positive definite again near the final stage. The bifurcation pattern and the corresponding bifurcation strain (7%) agree well with Yakobson *et al.*¹⁹ molecular mechanics studies.

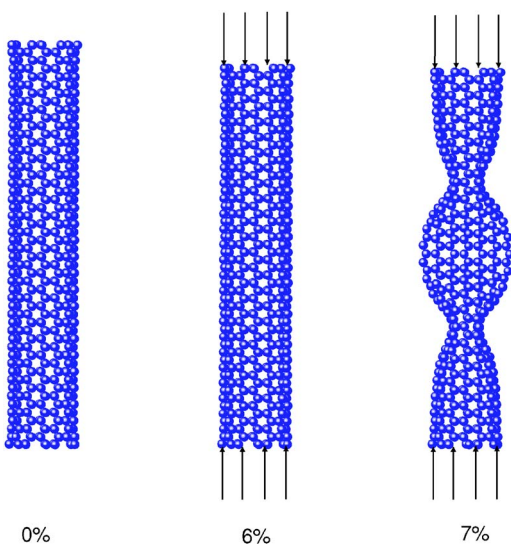


FIG. 7. (Color online) Deformation patterns for a 6-nm-long (7,7) carbon nanotube under compression predicted by the atomic-scale finite element method (AFEM). Bifurcation occurs at 7% compressive strain. This shows that AFEM is stable.

V. LINKING AFEM WITH CONTINUUM FEM

The main advantage of AFEM is that it can be readily linked with the conventional continuum FEM in a unified theoretical framework, thus provides a seamless computational method for multiscale simulation. The total energy in the system is minimized simultaneously with respect to both atom positions (in AFEM) and FEM nodes (in continuum FEM) in this unified theoretical framework. We have implemented this new AFEM element in the ABAQUS finite element program²⁰ via its USER-ELEMENT subroutine. We use a 605-nm-long (5,5) armchair CNT with 48 200 atoms in Fig. 8 to illustrate the combined AFEM/FEM. The CNT has two fixed ends, and is subject to a displacement of 81 nm in the middle, resulting in a 15° rotation at two fixed ends as in the Tomblor *et al.* experiment.²¹ Two computational schemes are adopted. In the first scheme [Fig. 8(a)], only AFEM elements are used and there are 48 200 elements. In the second scheme

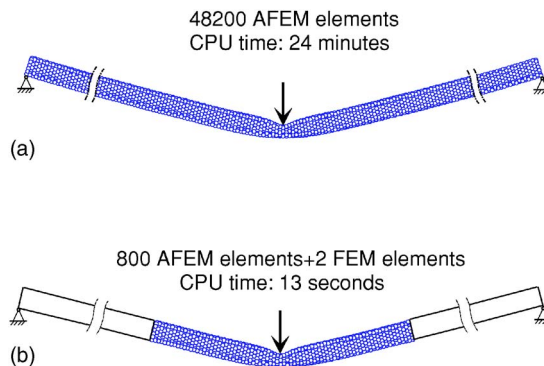


FIG. 8. (Color online) 605-nm-long (5,5) carbon nanotube with 48 200 atoms subject to 81 nm deflection in the middle. The atomic-scale finite element method (AFEM) takes 24 min to determine atom positions, while the combined AFEM/FEM takes only 13 s. This shows that the combined AFEM/FEM is an efficient multiscale computational method.

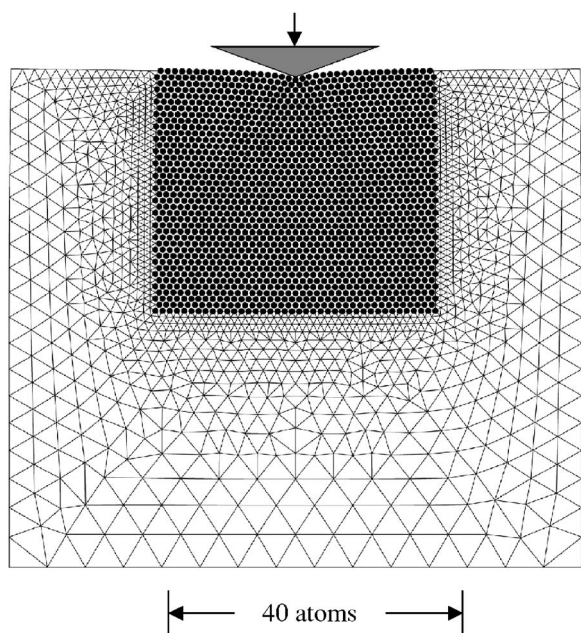


FIG. 9. Combined AFEM/FEM multiscale computation of 64 million atoms in a plane subject to nanoindentation. There are 1580 atoms and 2971 FEM nodes for the entire domain of computation, but only those near the nanoindenter are shown.

[Fig. 8(b)], AFEM elements are used for the middle portion of the CNT having 800 carbon atoms where deformation is highly nonuniform, while the rest of the CNT is modeled by conventional FEM elements; and two FEM string elements

are used, as shown in Fig. 8(b), with their tensile stiffness determined from the interatomic potential of carbon.²² The differences between results obtained from two schemes are less than 1%. However, the CPU time in the second scheme is only 13 s, which is less than 1% of that in the first scheme, 24 min. Moreover, the saving in computer memory is also tremendous since the second scheme requires less than 2% memory.

We have also used the combined AFEM/FEM to study the nanoindentation of a plane of 64 000 000 (8000 × 8000) atoms. The atoms have triangular lattice structure, and are characterized by the Lennard-Jones 6–12 potential. Figure 9 illustrates the computational scheme, which involves about 1600 atoms (i.e., 1600 AFEM elements) underneath the rigid indenter where the deformation is highly nonuniform, and about 3000 nodes for continuum finite elements (only a small portion of continuum elements are shown in Fig. 9). Here continuum finite elements are not applied to individual atoms (as discussed in Sec. II). Instead, they are applied to a continuum solid which has a constitutive model derived directly from the interatomic potential and triangular lattice structure.^{23,24} Near the AFEM/FEM boundary, the size of continuum finite elements is comparable to the atomic spacing to ensure the smooth transition from AFEM to FEM domains. We have also used a refined mesh which contains about 6400 atoms (i.e., 6400 AFEM elements) and the same number of continuum FEM nodes to ensure accuracy of results. The refined mesh gives the same results (e.g., atom positions underneath the indenter) as the mesh shown in Fig. 9.

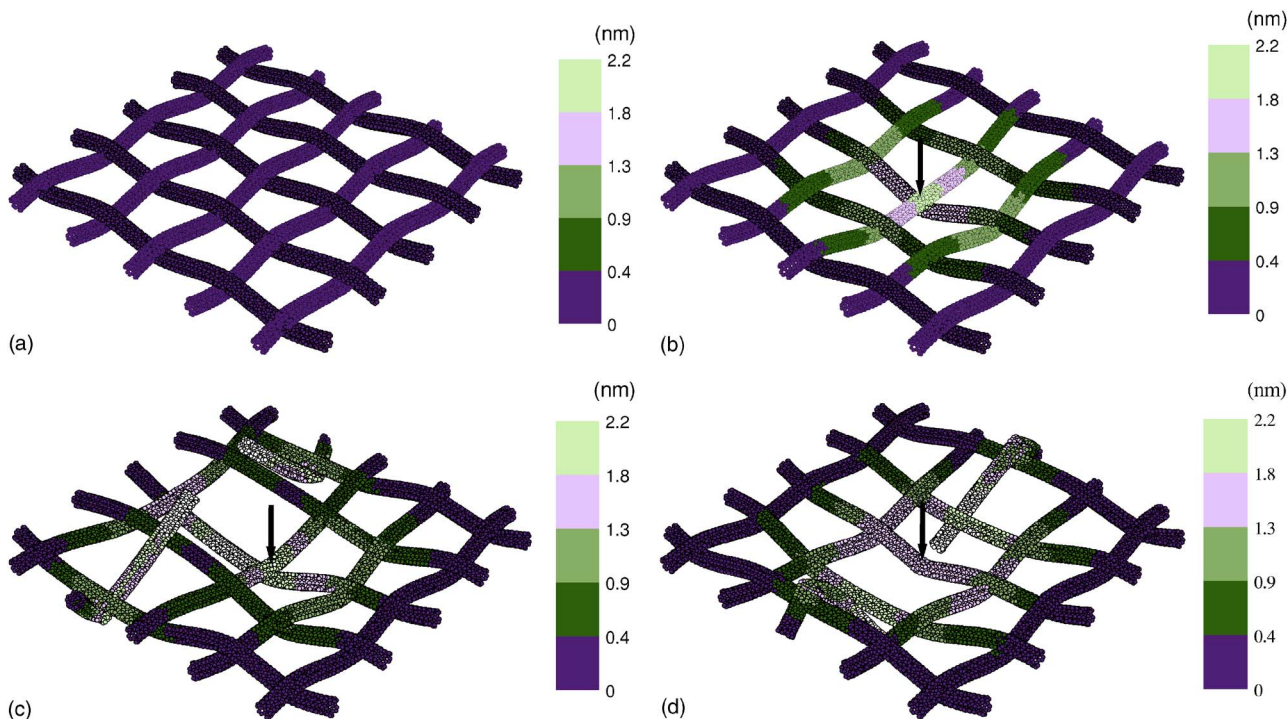


FIG. 10. (Color online) (a) Woven nanostructure of carbon nanotubes; (b) the woven nanostructure subject to a point force of 50 eV/nm as indicated; (c) the structure with a broken carbon nanotube away from the point force of 50 eV/nm; (d) the structure with a broken carbon nanotube underneath the point force of 50 eV/nm. The contours are used to distinguish displacements of atoms as shown with blue representing the neutral position and the red maximal deflection.

VI. APPLICATION OF AFEM TO WOVEN NANOSTRUCTURE OF CARBON NANOTUBES

Some complex atomic structures involving a large number of atoms with multiple kinds of atomistic interactions can be efficiently studied by AFEM on simple computational platforms such as personal computers.¹⁶ For example, structured composites possess designed mechanical, thermal, and electrical properties, and are provided in many forms in synthetic materials and exist in many biological systems in nature. The woven structure of CNT fibers has already been realized.²⁵ The woven nanostructure of individual CNTs, as shown in Fig. 10(a), is another representative candidate for exploiting the superior mechanical properties of CNT. It has the potential for unique applications, where ultimate toughness, strength and lightness are required, such as in body armor and aerospace product. Such a nanostructure is still difficult to assemble with the existing experimental technique, and is also a challenge for atomistic studies. Here we use AFEM to study this woven nanostructure of CNTs. Figure 10(a) shows ten (5,5) CNTs with 16 000 atoms that form a woven nanostructure with an intertube spacing of 3.86 nm. The interactions within the same CNT are characterized by Brenner's potential¹³ with the AFEM element in Fig. 1. Between CNTs, atoms interact through the van der Waals potential for carbon,²⁶ and nonlinear string elements incorporating such potential are used. The centers of end cross sections of all CNTs are on the same horizontal plane. Each end cross section has two atoms in the horizontal plane, and these atoms are fixed. The atomic structure shown in Fig. 10(a) corresponds to the relaxed, equilibrium state.

Figure 10(b) shows the deformed atomic structure subject to a vertical point force of 50 eV/nm at the center. The contours in Fig. 10(b) represent different levels of the displacements of atoms, where displacements are measured from the relaxed, equilibrium configuration in Fig. 10(a). The deflection, which is the displacement at the bottom of woven nanostructure (below the loading point), is 1.70 nm, while for comparison, the deflection in a single CNT subject to the same force (Fig. 4) is 3.08 nm, i.e., more than 80% larger. For the same structure subject to a lateral force of 50 eV/nm in the horizontal plane, the resulting displacement is 2.38 nm. Therefore, the woven nanostructure is much stiffer than a single CNT since all CNTs contribute to the stiffness.

We further examine the sensitivity of woven nanostructure to defects. Figure 10(c) shows the deformed atomic

structure, with one neighbor CNT broken. The structure is subject to the same vertical force of 50 eV/nm. The deflection is 2.01 nm, slightly larger than 1.70 nm for a perfect structure. In another case, where the top CNT underneath the force is broken, as shown in Fig. 10(d), the deflection is only 1.58 nm, which is even smaller than 1.70 nm for a perfect structure. This is because breaking of top CNT causes upward springback of the bottom CNT. This suggests that the woven nanostructure is insensitive to structural defects. If the woven structure involves more CNTs, it should have even higher stiffness and be less sensitive to defects.

VII. CONCLUDING REMARKS AND DISCUSSION

We have developed an atomic-scale finite element method (AFEM) which has exactly the same formal structure as continuum FEM, and therefore can be seamlessly combined with continuum FEM in multiscale computation. AFEM uses both first and second order derivatives of system energy, and is faster than the standard conjugate gradient method. For stable atomic structures and well-defined interatomic potentials, AFEM possesses order- N characteristics and is suitable for large scale problems, particularly after being combined with continuum FEM.

AFEM is applicable to many atomistic studies since it can incorporate other atomistic models such as tight-binding potential. Through continuous update of AFEM elements according to current positions of atoms, AFEM can also model the evolution of atomic structure. In fact, the string elements for van der Waals interaction are updated in the study of the woven nanostructure of CNTs in Fig. 10. We have already demonstrated that some rather complex problems can be studied via AFEM on a personal computer. Together with parallel computation technique, the combined AFEM/FEM is most effective for treating problems with a large number of degrees of freedom, and therefore significantly increases the speed as well as the system size in large scale computation. Many optimization problems involving a large number of variables can also be efficiently solved with AFEM if the corresponding \mathbf{K} (matrix of second-order derivatives) is sparse.

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¹F. F. Abraham, R. Walkup, H. Gao, M. Duchaineau, T. Diaz De La Rubia, and M. Seager, Proc. Natl. Acad. Sci. U.S.A. **99**, 5777 (2002).

²F. F. Abraham, R. Walkup, H. Gao, M. Duchaineau, T. Diaz De La Rubia, and M. Seager, Proc. Natl. Acad. Sci. U.S.A. **99**, 5783 (2002).

³G. E. Moore, Electronics **38**, 114, (1965).

⁴Stable atomic structure means no significant amount of atom bond breaking or formation of new bonds, while well-defined

interatomic potential refers to no drastic oscillatory behavior. These ensure that energy surface has no drastic changes and is smooth.

⁵R. E. Rudd and J. Q. Broughton, Phys. Status Solidi B **217**, 251 (2000).

⁶V. B. Shenoy, R. Miller, E. b. Tadmor, D. Rodney, R. Phillips, and M. Ortiz, J. Mech. Phys. Solids **47**, 611 (1999).

⁷S. Curtarolo and G. Ceder, Phys. Rev. Lett. **88**, 255504 (2002).

⁸W. E. and Z. Huang, Phys. Rev. Lett. **87**, 135501 (2001).

- ⁹H. Rafii-Tabar, L. Hua, and M. Cross, *J. Phys.: Condens. Matter* **10**, 2375 (1998).
- ¹⁰S. Kohlhoff, P. Gumbsch, and H. F. Fischmeister, *Philos. Mag. A* **64**, 851 (1991).
- ¹¹W. Yang, H. Tan, and T. F. Guo, *Modell. Simul. Mater. Sci. Eng.* **2**, 767 (1994).
- ¹²J. Tersoff, *Phys. Rev. Lett.* **61**, 2879 (1988).
- ¹³D. W. Brenner, *Phys. Rev. B* **42**, 9458 (1990).
- ¹⁴D. W. Brenner, O. A. Shenderova, J. A. Harrison, S. J. Stuart, B. Ni, and S. B. Sinnott, *J. Phys.: Condens. Matter* **14**, 783 (2002).
- ¹⁵W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes* (Cambridge University Press, New York, 1986).
- ¹⁶All computations are performed on a PC with 2.8 GHz CPU and 1 G memory.
- ¹⁷Corresponding CPU time is 24 min, which is about 50% longer than the linear projection from Fig. 4. This increase in CPU time is due to the reduced speed of data access in a PC for large problems.
- ¹⁸IMSL, IMSL(R) Fortran 90 MP Library Version 4.01, McGraw-Hill, San Ramon, 1999.
- ¹⁹B. I. Yakoboson, C. J. Brabed, and J. Bernholc, *Phys. Rev. Lett.* **76**, 2511 (1996).
- ²⁰ABAQUS, Inc. is the world's leading provider of software for advanced finite element analysis. The headquarter is located at 166 Valley St., Providence, RI 02909-2499.
- ²¹T. W. Tomblor, C. Zhou, L. Alexseyev, J. Kong, H. Dai, L. Liu, C. S. Jayanthi, M. Tang, and S. Wu, *Nature (London)* **405**, 769 (2000).
- ²²P. Zhang, Y. Huang, P. H. Geubelle, P. A. Klein, and K. C. Hwang, *Int. J. Solids Struct.* **39**, 3893 (2002).
- ²³B. Chen, Y. Huang, H. Gao, and W. Yang, *Int. J. Solids Struct.* **41**, 1 (2004).
- ²⁴B. Chen, Y. Huang, H. Gao, and P. D. Wu, *Int. J. Solids Struct.* **41**, 2293 (2004).
- ²⁵A. B. Dalton, S. Collins, E. Munoz, J. M. Razal, V. H. Ebron, J. P. Ferraris, J. N. Coleman, B. G. Kim, and R. H. Baughman, *Nature (London)* **423**, 703 (2003).
- ²⁶L. A. Girifalco, M. Hodak, and R. S. Lee, *Phys. Rev. B* **62**, 13104 (2000).