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Tailored metamaterials based on carbon nanotube nanotrusses: A molecular dynamics–neural network–finite element framework

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Abstract

The paper at hand deals with the optimal design of metamaterials. As a fundamental building block of such metamaterials, a nanotruss is used, preserving the benefits of classical macroscopic trusses. Each truss element is made of a single-walled carbon nanotube. Such a choice should ensure superior strength of this class of metamaterials. Due to the repetitive nature of the optimization process, a computationally efficient framework is required. On the other hand, molecular dynamics is considered to be the most accurate, albeit prohibitively slow for this purpose. To achieve this goal, machine learning is used. More specifically, a partially input convex neural network takes the role of a constitutive model for all single-walled carbon nanotube configurations of practical interest. This network also incorporates fundamental principles of physics. Convexity is included in the architecture of the neural network and addresses the issue of noise caused by temperature effects. It is important to emphasize that the neural network is trained on a dataset obtained by molecular dynamics, and thus retains the accuracy of molecular dynamics. The developed neural network is then coupled to the Abaqus finite element code, providing constitutive behavior to nonlinear finite element calculations. Finally, the framework is linked to the optimization code Indago. The performance of the framework is demonstrated on an example. It is concluded that the framework is computationally efficient, yet accurate. The strong nonlinear apparatus available in Abaqus ensures the versatility of the framework.

***Keywords**: single-walled carbon nanotubes; partially input convex neural networks; shape optimization; metamaterials; molecular dynamics.*

1. Introduction

Nowadays, the focus of many researchers is oriented toward the development of metamaterials with extreme material properties. The building blocks of such metamaterials usually are hierarchical nanotruss structures [1], made either of polymers or ceramics [1], or of carbon [2]. Using a truss structure as a building block ensures the well-known macroscopic engineering properties of trusses - used for thousands of years - as lightweight structures with high load capacity. The most intriguing property of such metamaterials is that they possess the strength of conventional steel, while having a specific mass density comparable to that of Styrofoam.

The present research considers single-walled carbon nanotubes (SWCNTs) as the truss elements. Although such structures have not yet been fabricated in laboratories, this academic study nevertheless aims to develop a computational framework that could be used to investigate them. The choice of SWCNTs is justified by molecular dynamics (MD) simulations of uniaxial tensile loading, which demonstrate that they possess theoretical ultimate tensile strengths up to 200 times greater than that of conventional structural steels [3]. Although the presence of defects - such as atomic vacancies, topological irregularities, and interfacial discontinuities - can significantly reduce their effective strength, SWCNTs still retain exceptional mechanical properties. This makes them promising candidates for reinforcing composite materials where both strength and weight savings are important. These nanocomposites are already finding application in lightweight, high-performance sporting equipment, as well as in the aerospace, automotive, and defense sectors.

Beyond the conventional use of single-walled carbon nanotubes (SWCNTs) as reinforcement in composite materials, as already indicated, this research aims to analyze

SWCNTs as fundamental components of nanotruss structures. However, a major bottleneck in the development and analysis of such SWCNT-based truss materials is the lack of an adequate computational framework. Several modeling strategies are available, but each has significant limitations:

- Molecular Dynamics (MD): MD simulations are often considered the most realistic due to the inclusion of atomic interactions and thermal effects. The methodology is now well-established for simulating mechanical problems at the nanoscale. Unfortunately, the computational cost of MD becomes prohibitive when applied to structures involving large numbers of atoms, such as those found in SWCNT-based trusses. This effectively rules out repetitive calculations, such as those required in optimization.
- Finite Element Method (FEM): FEM is often a straightforward choice and, in this context, is known as Molecular Structural Mechanics (MSM) [4, 5]. MSM models the carbon–carbon bonds in SWCNTs as beam finite elements with equivalent stiffnesses. The method is computationally efficient but is often restricted to linear formulations and offers significantly reduced accuracy compared to MD, even when nonlinearities are partially included. Furthermore, the method leads to a large number of elements, since each C-C bond must be explicitly modeled.
- Analytical Nonlocal Elasticity Models: Nonlocal continuum models attempt to capture nanoscale effects by introducing an additional length-scale (small-size) parameter [6]. This parameter extends the classical constitutive equations to account for atomic-scale interactions, i.e., small-size effects. This approach leads to mathematically sound beam models; however, it depends heavily on the precise value of the nonlocal parameter. This parameter is not easily determined—it can be obtained from MD or experimental data, but its small magnitude makes it highly sensitive to noise introduced by thermal vibrations in MD simulations or to measurement limitations in experimental setups. For this reason, most MD simulations are performed at 0 K. This remains a serious issue in the application to real engineering structures.

Thus, it is clear that all existing approaches suffer from serious drawbacks. For this reason, the present research proposes a fourth modeling strategy that combines the atomistic accuracy of MD with the efficiency of FEM. Each SWCNT is modeled as a single rod-like finite element, rather than using individual beam finite elements to represent atomic bonds. The small-size parameter will be included implicitly in the formulation, eliminating the need to incorporate it as a separate parameter explicitly. This is achieved by substituting the classical constitutive model with a neural network (NN). The NN will be trained on a large dataset obtained from MD simulations of uniaxial tension and compression of individual SWCNTs. This paper presents only the central ideas of the framework, while further details and examples can be found elsewhere [1, 8–10].

2. Molecular Dynamics – Uniaxial Tension and Compression Test of SWCNTs

In order for the NN to achieve the same reliability as MD, it is clear that it should be trained on data produced by MD. To this end, a comprehensive set of 818 different SWCNTs, including all possible configurations up to 4 nm in diameter, was prepared. The length-to-diameter ratio was approximately 5 in all cases. The SWCNT lengths ranged from 1.899 to 19.836 nm, while the smallest and largest configurations were (4,1) and (50,2) nanotubes, respectively. Tension and compression MD simulations were carried out using LAMMPS [11] at a temperature of 300 K. Note that introducing a temperature higher than 0 K causes stochastic vibrations of atoms, which in turn induce vibrations in the entire nanotube structure. Such vibrations can be regarded as unwanted noise inherently present in the results. To alleviate issues caused by stochastic vibrations associated with temperature, each test was performed three times, and the results were averaged. The main results were true stress - true strain curves for each SWCNT, evaluated under both tension and compression.

The governing potential was the modified AIREBO [12], which is often considered the most accurate among classical potentials. One end of each SWCNT was held fixed, while a velocity was prescribed at the other end such that the strain rate was 0.001 ps^{-1} for every SWCNT configuration considered. For further details, see [3, 8–10]. The equilibration time was 25 ps, and the time step was 0.5 fs.

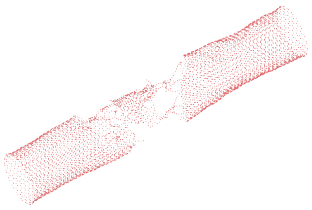


Fig. 1. Tensile fracture of (20,20) SWCNT

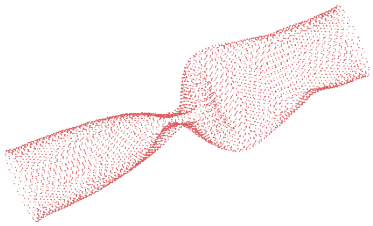


Fig. 2. Shell-like buckling of (20,20) SWCNT

3. Neural Networks and Convexity

The dataset obtained from MD simulations consisted of points, where each point was defined by the following data: true stress, true strain, and the chirality parameters n and m for the particular SWCNT. The complete dataset consisted of approximately three million points, or 3700 in average.

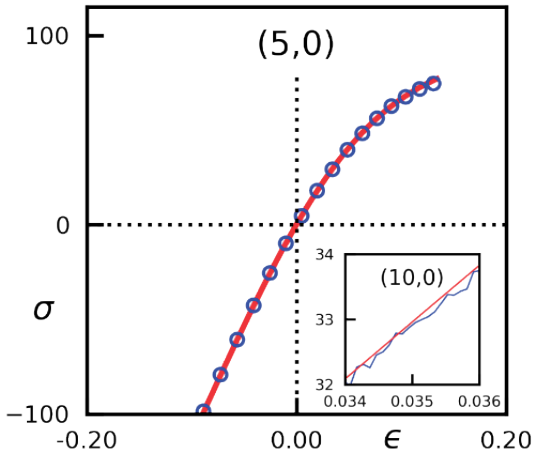


Fig. 3. True stress–true strain curve for a (5,0) SWCNT. The inset shows a detail of the stress–strain curve for a (10,0) SWCNT. The red curve represents results obtained by the NN, while the blue curve corresponds to the MD results. Stresses are given in GPa.

With this dataset at hand, a neural network was trained. Initial attempts [8], carried out with three different types of NNs, showed that all were able to capture stress-strain curves with remarkable accuracy. In particular, all noise induced by the stochastic vibrations related to temperature (blue line in the inset of Fig. 3) was reproduced by the NN. It is clear that the stresses do not monotonically increase with strain. This, in turn, leads to negative tangent moduli, which effectively rules out the application of such NNs in nonlinear finite element calculations due to convergence issues.

An additional problem stemming from the violation of monotonicity is the loss of convexity of the strain energy with respect to strain. Although the convexity requirement is often considered too strict [13, 14], it is necessary in the present one-dimensional case involving truss elements. For this reason, the neural network should be designed to ensure that the strain energy is convex with respect to strain. However, since the chirality parameters n and m are also inputs to the NN, convexity constraints should not be imposed on these parameters.

Feed-forward neural networks of this kind are known as partially input convex neural networks (PICINNs) and were first described by Amos et al. [15] in 2017. The same authors also introduced neural networks whose output is convex with respect to the entire input. The latter type of networks is now frequently used in computational mechanics [16–18], while PICINNs are less common [19]. The cornerstone of such networks relies on well-known theorems from convexity theory. In particular, a function is convex if it is a composition of non-decreasing convex functions and if it is a sum of non-negative convex functions. If an additional requirement is integrability, this leaves the Softplus activation function as the only choice. To summarize, a neural network designed in this manner is convex with respect to its input by design. Further modifications can make this network partially input convex [15, 9].

Additionally, it is advantageous to include other physics-based conditions in the design of the network. In particular, the PICINN described above requires that the strain energy be a convex function of strain. This implies that NN training should be performed using strain–energy pairs. Although the energy could be estimated from the available stress–strain data, this procedure would be cumbersome. To address this issue, the network is designed with strain (and chirality parameters) as inputs, and strain energy as the output. However, autodifferentiation capabilities are exploited so that training is performed on stress–strain pairs, a method known as Sobolev training. This means that stress is the first derivative of strain energy with respect to strain, automatically ensuring thermodynamic consistency. The approach also exactly satisfies the requirements that energy and stress vanish at zero strain. Finally, the growth condition (energy tending to infinity as strain tends to infinity) and the condition that energy is non-negative are also fulfilled. In the present case, the PICINN is developed using TensorFlow 2.

The trained PICINN can then serve as the constitutive model, providing strain energy and stresses for a given strain. Further differentiation also yields the tangent modulus. The final step is coupling the model to the UMAT subroutine in Abaqus, resulting in a very general framework suitable for solving a variety of nonlinear problems involving trusses. Such a procedure could not be performed with MD due to the exceptional computational costs involved. For comparison, a single SWCNT tensile test MD simulation lasted from 6 minutes for the smallest SWCNT to 6 hours for the largest one. Using the trained PICINN as a surrogate reduced this time to a fraction of a second. Thus, the present approach differs from the classical MSM approach. In the classical MSM approach, each rod (or, more commonly, beam) represents the forces between atoms. In contrast, in the present approach each rod represents an entire nanotube rather than the interaction between individual atoms. By adjusting the rod material properties using PICINN, an accurate yet computationally inexpensive method is obtained.

4. Optimization Framework

In the MD-NN-FEM framework presented here, the computational costs are reduced significantly. This, in turn, enables repetitive procedures like optimization to be carried out within a realistic timeframe. While the MD – NN - FEM framework provides a computational tool for simulating carbon nanotube - based nanotrusses, tailored properties of some metamaterials can be achieved through optimization. This can include reducing the weight of a nanostructure, maximizing the stored elastic energy in a metamaterial, minimizing the Poisson's ratio to obtain an auxetic material, or increasing the compressive strength. Other possibilities also exist.

The optimization tool used for the present study is Indago [20]. The optimization performed can be classified as shape optimization. In particular, several variables defining the geometry of the nanotruss are selected, and a mesh suitable for the Abaqus FEA code is produced. The methods used in this research were Nelder–Mead (NM)

[21], Particle Swarm Optimization (PSO) [22], Artificial Bee Colony optimization (ABC) [23], Squirrel Search Algorithm (SSA) [24], and Bat Algorithm (BA) [25]. The best global minimum was always obtained by the Nelder–Mead method, albeit at the cost of a higher number of optimization repetitions. PSO and SSA also demonstrated very good performance, while ABC and BA showed inferior results.

5. Example

As an illustration of the framework's performance, an energy-trapping metamaterial is considered. The nanotruss based on SWCNTs is motivated by the research in [26], where bi-stable structures were studied. While in [26] beams connecting two rigid layers buckle elastically and can assume a second stable configuration, in the present case, a nanotruss replaces the beam (Fig. 4). Note that the stored energy can be recovered by reversing the direction of the load.

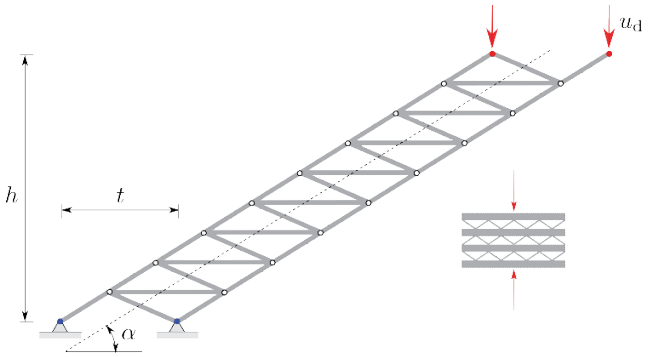


Fig. 4. Basic building element of an energy trapping metamaterial, along with the variables used in optimization.

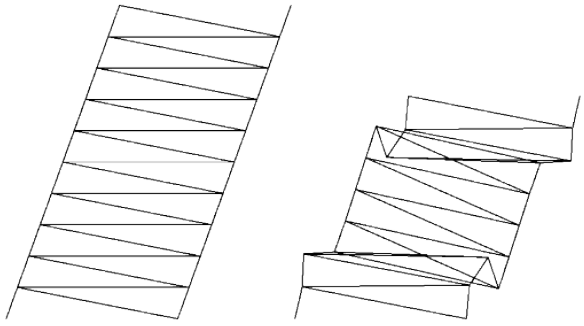


Fig. 5. Initial and final configuration of an energy trapping nanotruss.

Shape optimization was performed to find the variables t, h and α that produce a structure capable of storing as much energy as possible. Constraints were imposed on the allowable stresses, as well as on the maximum length of each SWCNT, which was limited to no more than 12.5 times its diameter. This latter constraint ensured that beam-like buckling of each nanotube could not occur. The nanotruss was made of (7,0) SWCNTs.

Global optimum was obtained for t=4.534 nm, h=8.257 nm, α=70.048° while stored energy was 37.98 nN nm, Fig. 5. The final configuration shows that a rigid rotation of the central part of the nanotruss occurs, effectively locking the stored energy.

For more details, see [10].

6. Concluding Remarks

The research presented a tool that maintains simulation costs at the level of finite element analysis while preserving the accuracy of molecular dynamics. This outcome was achieved through the application of feed-forward neural networks that serve as the constitutive model.

However, straightforward use of a standard feed-forward neural network is not possible; instead, one must rely on the PICINN extension, incorporating fundamental physics constraints directly into the NN architecture. The PICINN was coupled to the standard FEM code Abaqus, thereby ensuring both the generality of the approach and the availability of Abaqus's robust numerical capabilities.

Finally, the MD-NN-FEM procedure was coupled to the optimization code to enable the design of metamaterials with tailored properties.

The example demonstrated the applicability and efficiency of the developed framework. This versatile framework can be applied to any problem involving the optimal design of carbon nanotube–based nanotrusses.

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