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Scalable Nanohelices for Predictive Studies and Enhanced 3D Visualization

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Corresponding Author:	Lilian P. Davila, Ph.D. University of California Merced Merced, CA UNITED STATES
Corresponding Author Secondary Information:	
Corresponding Author E-Mail:	ldavila@ucmerced.edu
Corresponding Author's Institution:	University of California Merced
Corresponding Author's Secondary Institution:	
First Author:	Kwyn A. Meagher, B.S.
First Author Secondary Information:	
Other Authors:	Kwyn A. Meagher, B.S.
	Benjamin N. Doblack, M.S.
	Mercedes Ramirez, B.S.
Order of Authors Secondary Information:	
Abstract:	Spring-like materials are ubiquitous in nature and of interest in nanotechnology for energy harvesting, hydrogen storage, and biological sensing applications. For predictive simulations, it has become increasingly important to be able to model the structure of nanohelices accurately. To study the effect of local structure on the properties of these complex geometries one must develop realistic models. To date, software packages are rather limited in creating atomistic helical models. This work focuses on producing atomistic models of silica glass (SiO_2) nanoribbons and nanosprings for molecular dynamics (MD) simulations. Using an MD model of "bulk" silica glass, two computational procedures to precisely create the shape of nanoribbons and nanosprings are presented. The first method employs the AWK programming language and open-source software to effectively carve various shapes of silica nanoribbons from the initial bulk model, using desired dimensions and parametric equations to define a helix. With this method, accurate atomistic silica nanoribbons can be generated for a range of pitch values and dimensions. The second method involves a more robust code which allows flexibility in modeling nanohelical structures. This approach utilizes a C++ code particularly written to implement pre-screening methods as well as the mathematical equations for a helix, resulting in greater precision and efficiency when creating nanospring models. Using these codes, well-defined and scalable nanoribbons and nanosprings suited for atomistic simulations can be effectively created. An added value in both open-source codes is that they can be adapted to reproduce different helical structures, independent of material. In addition, a MATLAB graphical user interface (GUI) is used to enhance learning through visualization and interaction for a general user with the atomistic helical structures. One application of these methods is the recent study of

	nanohelices via MD simulations for mechanical energy harvesting purposes.
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June 29, 2013

Dear Editor:

Please find enclosed a manuscript entitled "*Bottom-up approach to atomistic modeling of helical nanostructures for molecular dynamics simulations via scalable open-source coding*," by Meagher, Doblack, Ramirez and Davila which we are submitting for your consideration to be published in the *Journal of Visualized Experiments (JoVE)*.

In this paper we report the successful modeling of helical nanostructures using open-source codes for molecular dynamics (MD) simulations, and a graphical interface to enhance research and learning through visualization. Modeling the atomistic structure of nanohelices accurately is becoming increasingly important in predictive simulation studies toward materials research and novel nanotechnology applications involving energy harvesting, biological sensing, hydrogen storage, and many others. To understand the effect of local structure on the mechanical properties of these novel materials, we need to produce nanohelical models which can be accurately and efficiently created. To date, software packages are rather limited in the ability to create atomistic helical models. Recent related research using these helical models has been published and has been included as a reference.

We believe this paper makes an important contribution to the science community since it: 1) facilitates the efficient modeling of nanohelices for MD simulations for promising novel applications, 2) disseminates results via an open-source code (NanospringCarver) to be distributed broadly through my research group's website, 3) promotes efficient atomistic simulations which can be pursued on varied computing platforms, 4) contains outcomes which have been reported in large-scale MD simulations to study the mechanical properties of silica nanohelices, 5) expands the number of learning tools for computational classes via the designed MATLAB GUI, and 6) promotes collaborations and interdisciplinary projects.

Although there are some articles on simulations of helical structures in the literature, there is little or no information about the methods used to create the limited number of helical models reported to date. We believe our study is unique in that it involves the development and presentation of robust and adaptable codes which can be used in atomistic simulations, and a MATLAB GUI to enhance visualization.

Performing MD simulations to study the response of helical structures to different loading conditions is feasible with accurate atomistic models and appropriate interatomic potentials. The success of future manufacturing using nanostructures will depend on understanding their physical properties, with implications on self-assembly and nanomanipulation processes. This work is a step towards understanding the behavior of such nanostructures using MD simulations.

We believe that *Journal of Visualized Experiments* is the most suitable journal to publish this work because of its unique multimedia format, and since our results are highly visual in nature and can be applicable to other similar systems. The computational results from this study can be compared to those obtained through experimental studies using AFM or TEM. Hence, the work presented in this paper is important to a broad group of scientists and specialists in nanoscience and nanotechnology.

We hope you find our paper interesting and worth publishing in your journal. We look forward hearing from you soon. Thank you for your consideration.

Sincerely,

Lílian P. Dávila, Ph.D., Assistant Professor
Materials Science and Engineering, University of California, Merced
e-mail: ldavila@ucmerced.edu, Phone: (209) 228-4707

Author contributions:

Kwyn A. Meagher
Created nanoribbon open-source code, contributed to manuscript (figures).

Benjamin N. Doblack
Created nanospring open-source code, contributed to manuscript (figures, videos, manual).

Mercedes Ramirez
Created MATLAB graphical user interface, contributed to manuscript (figures, manual).

Lilian P. Dávila
Created and led project, supervised students, contributed with initial bulk glass model, prepared manuscript and supplementary documentation.

Name of JoVE editor who assisted me in the submission process:

Rachelle Baker
Associate Editor – Physical Sciences, JoVE
e-mail: rachelle.baker@jove.com

Peer reviewer's names and institutional affiliation and email addresses:

Prof. James Shackelford
University of California Davis
e-mail: jfshackelford@ucdavis.edu

Prof. Mark Asta
University of California Berkeley
e-mail: mdasta@ucberkeley.edu

Prof. Maria J. Caturla
University of Alicante, Spain
e-mail: mj.caturla@ua.es

Prof. Stephen H. Garofalini
Rutgers University
e-mail:shg@rutgers.edu

Prof. Subhash Risbud
University of California Davis
e-mail: shrisbud@ucdavis.edu

Prof. Sabyasachi Sen
University of California Davis
e-mail: sbsen@ucdavis.edu

Title:
Scalable Nanohelices for Predictive Studies and Enhanced 3D Visualization

Authors:
Kwyn A. Meagher[1], Benjamin N. Doblack[1], Mercedes Ramirez[2], and Lilian P. Dávila[1,*]
[1]Materials Science and Engineering, School of Engineering
[2]Computer Science and Engineering, School of Engineering
University of California Merced, 5200 N. Lake Road, Merced, CA 95343, U.S.A.

Corresponding Author:
Lilian P. Dávila, University of California Merced, ldavila@ucmerced.edu, phone (209) 228-4707

Keywords:
Helical atomistic models; open-source coding; graphical user interface; visualization software; molecular dynamics simulations; graphical processing unit accelerated simulations.

Short Abstract:
Accurate modeling of nanohelical structures is important for predictive simulation studies leading to novel nanotechnology applications. Currently, software packages and codes are limited in creating atomistic helical models. We present two procedures designed to create atomistic nanohelical models for simulations, and a graphical interface to enhance research through visualization.

Abstract:
Spring-like materials are ubiquitous in nature and of interest in nanotechnology for energy harvesting, hydrogen storage, and biological sensing applications. For predictive simulations, it has become increasingly important to be able to model the structure of nanohelices accurately. To study the effect of local structure on the properties of these complex geometries one must develop realistic models. To date, software packages are rather limited in creating atomistic helical models. This work focuses on producing atomistic models of silica glass (SiO_2) nanoribbons and nanosprings for molecular dynamics (MD) simulations. Using an MD model of "bulk" silica glass, two computational procedures to precisely create the shape of nanoribbons and nanosprings are presented. The first method employs the AWK programming language and open-source software to effectively carve various shapes of silica nanoribbons from the initial bulk model, using desired dimensions and parametric equations to define a helix. With this method, accurate atomistic silica nanoribbons can be generated for a range of pitch values and dimensions. The second method involves a more robust code which allows flexibility in modeling nanohelical structures. This approach utilizes a C++ code particularly written to implement pre-screening methods as well as the mathematical equations for a helix, resulting in greater precision and efficiency when creating nanospring models. Using these codes, well-defined and scalable nanoribbons and nanosprings suited for atomistic simulations can be effectively created. An added value in both open-source codes is that they can be adapted to reproduce different helical structures, independent of material. In addition, a MATLAB graphical user interface (GUI) is used to enhance learning through visualization and interaction for a general user with the atomistic helical structures. One application of these methods is the recent study of nanohelices via MD simulations for mechanical energy harvesting purposes.

Introduction:
Helical nanostructures are typically produced in the laboratory using chemical vapor deposition techniques[1-2], while new approaches have been reported in the literature[3]. In particular nanosprings and nanoribbons have been studied because of their distinct properties and promising applications in sensors, optics, and electromechanical and fluidic devices[4-7]. Synthesis methods have been reported to produce silica (SiO_2) nanoribbons, making these structures potential building block units for hierarchical systems. Novel synthesis of 3D silica nanosprings has expanded their applications to chemiresistors when coated with ZnO[8] or nanoparticles for diagnostic applications[9-10].

Experimental studies on the mechanical properties of silica nanosprings and nanoribbons are scarce, primarily due to current limitations in manipulation and testing methods and equipment. Investigations into the nanomechanics of nanostructures and nanosprings have been reported using theory and simulations[11-14]. Some simulations[13] have focused on nanomechanical behavior of amorphous nanosprings because they can explore regimes not fully accessible through experimentation. Atomistic studies of metallic nanosprings have been reported in literature to investigate the size dependence of elastic properties[15], and more recently the nanomechanics of helical crystalline silica nanostructures[14]. Experimental testing of nanospring structures has also been performed in different materials such as helical carbon nanostructures and carbon nanocoils[16-17]. Despite the knowledge gathered thus far, a more complete understanding of the mechanical properties of these novel nanostructures is needed for future nanodevice fabrication efforts.

As MD studies of silica glass (non-crystalline silica) nanohelices are still quite limited, the atomistic modeling of such structures requires the creation of customized codes. No other alternative methods of creating silica glass helical MD models have been identified thus far upon recent literature search. In this work, a bottom-up approach to the atomistic modeling of helical silica glass nanostructures including nanosprings and nanoribbons is pursued for future large-scale MD nanomechanical simulations. The general approach involves the creation of an MD "bulk" silica glass model as reported previously[18], and carving out various helical nanostructures from this "bulk" sample via two robust and adaptable computer codes developed for this purpose. Both computational procedures offer a distinct way to create nanoribbon and nanospring models with great efficiency and atomistic detail; these structures are suitable for large-scale atomistic simulations. In addition, a customized graphical user interface is used to facilitate creation and visualization of the helical structures.

The structure of the "bulk" silica glass model is initially created at room temperature. Large-scale MD simulations are conducted for this purpose using the Garofalini interatomic potential similar to prior studies[18], which is relatively efficient computationally and appropriate for large systems. The initial "bulk" silica glass structure consists of a cubical model (14.3 x 14.3 x 14.3 nm^3) which contains 192,000 atoms. The "bulk" silica glass model is equilibrated at 300K for 0.5 ns to obtain the initial state using periodic boundary conditions.

Two computational procedures are designed and utilized to create atomistic silica nanoribbon and nanospring models. The first method involves carving out silica nanoribbons from the "bulk" structure using the parametric equations that define a helix, and its geometry (pitch,

radius of helix, and wire radius). This procedure includes using the AWK programming language, the LINUX operating system, and open-source visualization software[19]. The general iterative procedure to create atomistic models of nanoribbons involves: (1) selecting an atom in the "bulk" silica glass model, (2) calculating the distance from the selected atom to a point in space on a pre-defined helical function, (3) comparing this distance to the radius of the desired nanoribbon, and (4) discarding or keeping the atom in an output data model. A detailed step-by-step description for this method is included in the **Scalable Open-Source Codes Supplemental Material**. With this method, several silica nanoribbons were created using different pitch, radius of helix and nanoribbon radius values, which were measured subsequently for accuracy against the desired dimensional values with molecular analysis and visualization software[19-20]. Atomistic models of silica nanoribbons were generated with functional geometries (high values of pitch and low values of nanoribbon radius). Some artifacts, consisting of atoms excluded in error, leading to a less smooth nanoribbon surface, were observed at exceedingly high nanoribbon radius values and extremely low pitch values. Similar methods have been used in the process of creating silica nanowires[21-23].

The second method presented here includes carving out silica nanosprings from the "bulk" silica structure by implementing pre-screening methods to increase efficiency in addition to the mathematical equations for a helix. This procedure required creating a more robust C++ code to allow greater flexibility in modeling these helical nanostructures. The iterative method to create atomistic models of nanosprings includes: (1) discarding all atoms guaranteed to fall outside the helical path, (2) deterministically selecting a point on the helical path, (3) comparing all atoms within a specific distance to this selected point, and (4) discarding or storing each atom in an output data model. A step-by-step description for this method is also included in the **Scalable Open-Source Codes Supplemental Material.** With this method, several silica nanospring models were obtained with varied dimensions (wire radius, radius of helix, and pitch of nanospring) as shown in **Figure 1**. Highly precise silica nanospring models were obtained efficiently with this method, with no evidence of artifacts found at extreme (low and high) pitch values for the nanospring. The creation and use of the graphical user interface for this method is described in the **Protocol** section.

[Insert here: Figure 1]

This protocol describes how to prepare the NanospringCarver files, running MATLAB[24] on a LINUX[25] PC, and use a graphical user interface to prepare atomistic nanospring models. These previously unavailable models serve as the basis for novel molecular dynamics (MD) simulations[23] toward materials innovation research.

The general step-by-step procedure to create atomistic nanospring models involves using the following elements: (a) NanospringCarver (v. 0.5 beta) code (open-source in C++ language), (b) bulk silica glass model (input file), (c) MATLAB GUI interface and related files, and (d) MATLAB software (version 7) using a local license on a LINUX PC. Items (a)-(c) above (NanospringCarver code, silica glass model, MATLAB GUI files) are free to download online[26]. MATLAB (Matrix Laboratory) is a high-level language for numerical computation, visualization, and application development from MathWorks[24], which is mostly used for data visualization and analysis, image processing, and computational biology.

Protocol:

1. Preparing NanospringCarver files and starting MATLAB on a LINUX PC

The following steps are designed for a general user to make use of the files provided online[26].

1.1. Unpack the **nanosprings.tar.gz** file archive into the "Home" or another preferred directory.

1.1.1. Download the **nanospring.tar.gz** file archive from the web repository[26].

1.1.2. Locate the downloaded archive and move it to a preferred working directory entitled "Documents/Nanosprings".

1.1.3. Right-click **nanosprings.tar.gz** and select "extract here" from the right-click context menu.

1.2. Verify that all of the required files are present in the current directory. A list of those files and their purpose follows:

Makefile – manually managed compile file for nanosprings.cpp and Point.cpp
Nanosprings.fig –MATLAB GUI internals
Nanosprings.m –MATLAB GUI code
Point.cpp – Point (atom) class definition
Point.h – Point (atom) class header
carve – stand-alone nanosprings executable
example.par – example parameter file
glasscube.inp – glasscube data file
nanosprings.cpp – main nanosprings code
nanosprings_diagram.jpg – example nanospring for display
nanospringsmex.cpp – MATLAB-integrated nanosprings.cpp
nanospringsmex.mexglx – MATLAB-integrated nanosprings executable

Note: The user will need to create the "**nanospringsmex.mexglx**" executable file for the particular Linux machine being used (32-bit version in this example). If this has not yet been done, verify access to the MATLAB "mex" compiler by typing on the command line "**which mex**" and verifying the existence of the program. Also verify access to the MATLAB program by typing on the command line "**which matlab**". Using a command line to type "**mex nanospringsmex.cpp Point.cpp**" will create the "**nanospringsmex.mexglx**" executable MATLAB-integrated NanospringCarver file, as shown in the instructions below. Though not required for the GUI interface, if desired a stand-alone version of the NanospringCarver program can be created by typing "**make**" on a command line. This will compile the **nanosprings.cpp** and **Point.cpp** program elements together to create the "**carve**" executable file. In this tutorial, the "**glasscube.inp**" file contains position information for 192,000 silicon and oxygen atoms representing a silica glass model, with each line containing an atom ID, atom type, and x, y, z coordinates for the atom. The first line of the file is the total atom count (192000). The atomic

coordinates in this file are relative values, which if multiplied by 0.716 would represent nanometer distances.

1.3. On the desktop, open a terminal window. On many LINUX versions accomplish this by simultaneously pressing the "Ctrl", "Alt" and "T" keys.

1.4 Change the directory to the folder into which the nanosprings project files were extracted by typing:

cd Documents/Nanosprings/

1.5. Next, run the command to compile the binary for the system by typing:

mex nanospringsmex.cpp Point.cpp

1.6. Next initiate MATLAB by typing **matlab** on the command line

2. Modifying and using a graphical user interface (GUI) to the NanospringCarver program

Follow the steps below using the files provided online[26].

2.1. Open the GUIDE in MATLAB by clicking the GUIDE icon, on the top left toolbar area (**Figure 2**), to display a new window with the GUIDE quick start (**Figure 3**).

[Insert here: Figure 2.]

[Insert here: Figure 3.]

2.2. Use the "Open Existing GUI" tab (**Figure 4**) to modify an existing figure. Click on the "Browse" button to search for the existing GUI figure to be modified. After selecting the figure file (**Nanosprings.fig,** see blue box), click on "Open" on both windows to display a new window with the GUI figure. Locate the buttons available to be utilized for GUI creation on the left panel (**Figure 5**).

[Insert here: Figure 4.]

[Insert here: Figure 5.]

2.3. In order to run the GUI, click on "Run" under the "Tools" menu. Then, click "Yes" when a pop-up window prompts whether to save the figure before running. A new window displays the modified GUI**.**

2.4. If necessary, create another GUI for a different specific material using this GUI as an example.

2.5. To set up the example run, first click on the "Select input model file" button at the top of the GUI and navigate to the "**glasscube.inp**" file. Select this file and click "Open" to close the browsing window. The selected input file and path to it should now appear in the GUI window to the right of the "Selected input model file" button (**Figure 6**).

[Insert here: Figure 6.]

2.6. Next, use the "Browse" button in the "Output Model" section to browse for and select the directory to save the output model into. Ensure that the output directory is actively selected in order for the run to be enabled, even though there is an output directory already listed in the accompanying window to the right of this button.

Note: The "Advance Parameters Minimum Distance" value listed (0.209311 in **Figure 6**) was computed specifically for the "**glasscube.inp**" input file provided in this example, and should be left as is. This value may be computed as necessary on first use of a different input file by entering a value of "0" in this location before running the model. In this example, all parameter values are in relative units to match the input atomic coordinate system. If multiplied by 0.716 the parameter values would represent nanometer distances.

2.7. Run the example using the given spring parameters of $r = 1.0$, $R = 5.0$, $p = 1.5$, and $d = .209311$ by pressing the GUI "Run" button. View feedback from the run in the MATLAB Command window (**Figure 7**). In the feedback, check that the spring parameters are confirmed, that the input data file is read successfully, and the results stored in the output file named "**model**" are described.

[Insert here: Figure 7.]

Note: In the above example, the file "**model**" contains 5176 atoms comprising the desired spring, one per line, with the first line giving the total number of atoms in the file. Each line defining an atom includes the atom ID, atom type, and x, y, z coordinates of that atom.

2.8. Once the GUI interface is finalized, perform successive runs by right-clicking on "**Nanosprings.m**" in the MATLAB "Current Folder" window, and selecting "Run" to bring up the GUI interface directly.

Note: Various references are listed[27-31] for additional information on MATLAB GUIDE and the basic GUIDE interface.

3. Verifying NanospringCarver results in an open-source visualizer[19]

The following steps are designed for a general user to visualize and verify the output spring models created by NanospringCarver.

3.1. Use the NanospringCarver MATLAB GUI as described above to generate files for input into the visualization program[19]. When running the visualization program, use the "point

coordinate file" input option, distinguish atom types by color, and select an axis grid border for the field.

3.2. Measure distances in the spring models and make a record of them.

3.3. Compare measured data against desired spring dimensions and verify spring model accuracy.

4. Using NanospringCarver results in MD tensile simulations of nanosprings

The following steps are summarized for a general user to use the spring models created by NanospringCarver as input to a conventional open-source MD code[32].

4.1. Download the latest version of the open-source MD program LAMMPS. Refer to the associated online documentation for manuals and examples.

4.2. Determine the dimensions of the desired nanospring model in order to prepare the appropriate initial bulk silica glass model, as reported before[18].

4.3. Create the desired nanospring model using the NanospringCarver MATLAB GUI (see Section 2 above).

4.4. Perform tensile simulations on the desired nanospring, by stretching the model axially [11,13,23]. Produce a representative video of nanospring model being stretched (see **Figure 8,** below, and **Animated Fig1**) for visualization and analysis. Scientific results regarding the stress-strain behavior and stiffness of several nanospring models under tension have been reported elsewhere[23].

[Insert here: Figure 8.]

Representative Results:

The atomistic nanoribbon models created with the first computational procedure (nanoribbons code) and their associated dimensions are shown in **Figure 9**. The resulting nanospring models using the second computational procedure (nanosprings code) and associated dimensions are shown in **Figure 10**.

[Insert here: Figure 9.]

[Insert here: Figure 10.]

The range of nanoribbon and nanospring dimensions generated with both codes was ample (r < 3.75 nm, R < 9 nm, and p < 12.57 nm). Each of the above methods offers a unique way to create silica nanosprings and nanoribbons suitable for atomistic simulations. Both methods are flexible and can be adapted to produce different helical structures independent of the material, which makes them highly useful and versatile.

Table and Figure Legends:

Figure 1. A general helical structure showing characteristic dimensions, where *r*, *R* and *p* represent the wire radius, radius of helix, and pitch respectively. *H* denotes the total height of the helical structure[23].

Figure 2. MATLAB user interface showing how to open MATLAB GUIDE.

Figure 3. MATLAB GUIDE interface initializing.

Figure 4. MATLAB GUIDE interface showing how to open an existing GUI figure file.

Figure 5. MATLAB GUIDE interface showing tools for modifying an existing GUI figure.

Figure 6. Screenshot of using GUI to create an example silica nanospring model.

Figure 7. MATLAB Command window feedback from GUI-based Nanosprings run.

Figure 8. Screenshot of a silica nanospring during tensile simulation (see also Animated Fig1).

Figure 9. Atomistic model of a silica nanoribbon with desired dimensions: *r* (nanoribbon radius) = 1.07 nm, *R* (radius of helix) = 5.37 nm, and *p* (pitch) = 7.16 nm. Snapshots illustrate distinct views of the nanostructure: (a) top view, (b) lateral view, (c) lateral view with additional rotation, and (d)-(f) diagonal views. The SiO_2 nanoribbon model contains 3,354 atoms. The total ribbon height *H* is 14.1 nm[23].

Figure 10. Atomistic model of a silica nanospring with specified dimensions: *r* (wire radius) = 1.07 nm, *R* (radius of helix) = 4.29 nm, and *p* (pitch) = 4.29 nm. Snapshots show different views of the nanospring model: (a) top view, (b) lateral view, (c) lateral view with additional forward rotation, and (d)-(f) diagonal views. The SiO_2 nanospring model consists of 21,246 atoms. The total spring height *H* is 14.32 nm[23].

Animated Figure 1. Silica nanospring during tensile simulation.

Discussion:

Modification of the original approach to create nanohelical structures led to the development of two distinct codes to allow creation of both nanoribbons and nanosprings from an initial bulk silica glass MD model. The verification of the silica nanoribbon and nanospring models was pursued using different software packages[19-20], which confirmed their dimensional accuracy within the measurement capability of the programs. Comparison between nanosprings and nanoribbons was also performed by overlaying the models from different sides and angles, which resulted in additional geometry verification. Both computational methods developed in this project created helical nanostructures in a distinct way, with added value due to their scalability for use with any bulk material model size and potential use in modeling nanohelical structures from other materials. The resultant models presented here showed there are no detectable

artifacts (atoms missing from the desired nanohelical structure) generated using either method. In addition, the computational methods developed in this work are flexible for creating right-handed or left-handed helical nanostructures, simply by inverting the order of the sine and cosine functions defining the helix. Future applications of this method will include scaling to larger helical structures allowing extended parameter variation, and exploration of use with different initial materials.

Limitations of this method include dimensional restrictions on the created nanohelices depending on the initial bulk silica model used, which can involve significant computing resources as the model size increases. As currently implemented, the nanoribbon or nanospring height will extend to the size of the original bulk model. The first computational method generates accurate nanoribbon models for a range of parameters when the pitch value is greater than 7.16 nm and the radius of the helical wire is greater than 10% of the shortest dimension of the "bulk" silica glass structure. The second computational method generates accurate nanospring models without parameter limitation. This is particularly important for conducting MD simulations where readily available atomistic nanostructural models are needed to investigate different size conditions.

A critical step in the protocol would be to verify on first use of a particular initial MD bulk material model that the minimum distance between the closest two atoms in the model has been determined and input correctly with the dimensional parameters. Additionally, care should be taken to ensure that requested helical dimensions do not exceed the bulk material model dimensions.

Technological advances have facilitated the creation and characterization of complex helical nanostructures such as oxide nanoribbons and nanosprings in the laboratory. These nanoscale structures have unique properties that require thorough investigation in order to realize their full potential for various applications. MD studies of the mechanical behavior of these helical structures require flexible codes which can easily and precisely create helical nanostructures, and subsequently make use of appropriate interatomic potentials and methods for predictive simulations. To fulfill this first requirement, accurate structural modeling codes were developed which will be used for large-scale MD compression simulations and experimental validation.

This method of creating MD silica glass (non-crystalline) nanohelical models is significant, as similar codes not readily available and other alternative approaches have been focused on crystalline nanostructures. This modeling effort has been expanded, with the resultant nanostructures used in MD simulation studies, which have led to a thesis focused on the elastic response of silica glass nanohelices under tensile loads[23]. Time-efficient simulation of nanostructures is a challenging problem, however new programming techniques and atomistic models are especially becoming important for predictive studies. This modeling technique is rapidly gaining interest and quickly becoming an efficient method for models which require high performance computing. Future academic efforts will likely include the adaptation of these codes for training computational researchers and in classroom exercises. Performing MD simulations to study the response of helical structures to different loading conditions is certainly feasible with these robust atomistic models. The success of future manufacturing using these nanostructures as building blocks will depend on understanding of their structure and properties,

with implications on nanomanipulation and self-assembly processes. This work is a step toward understanding the mechanical behavior of such nanostructures using large-scale MD simulations, which can be potentially useful for designing nanodevices for a large number of applications.

Disclosures:
The authors declare that they have no competing financial interests.

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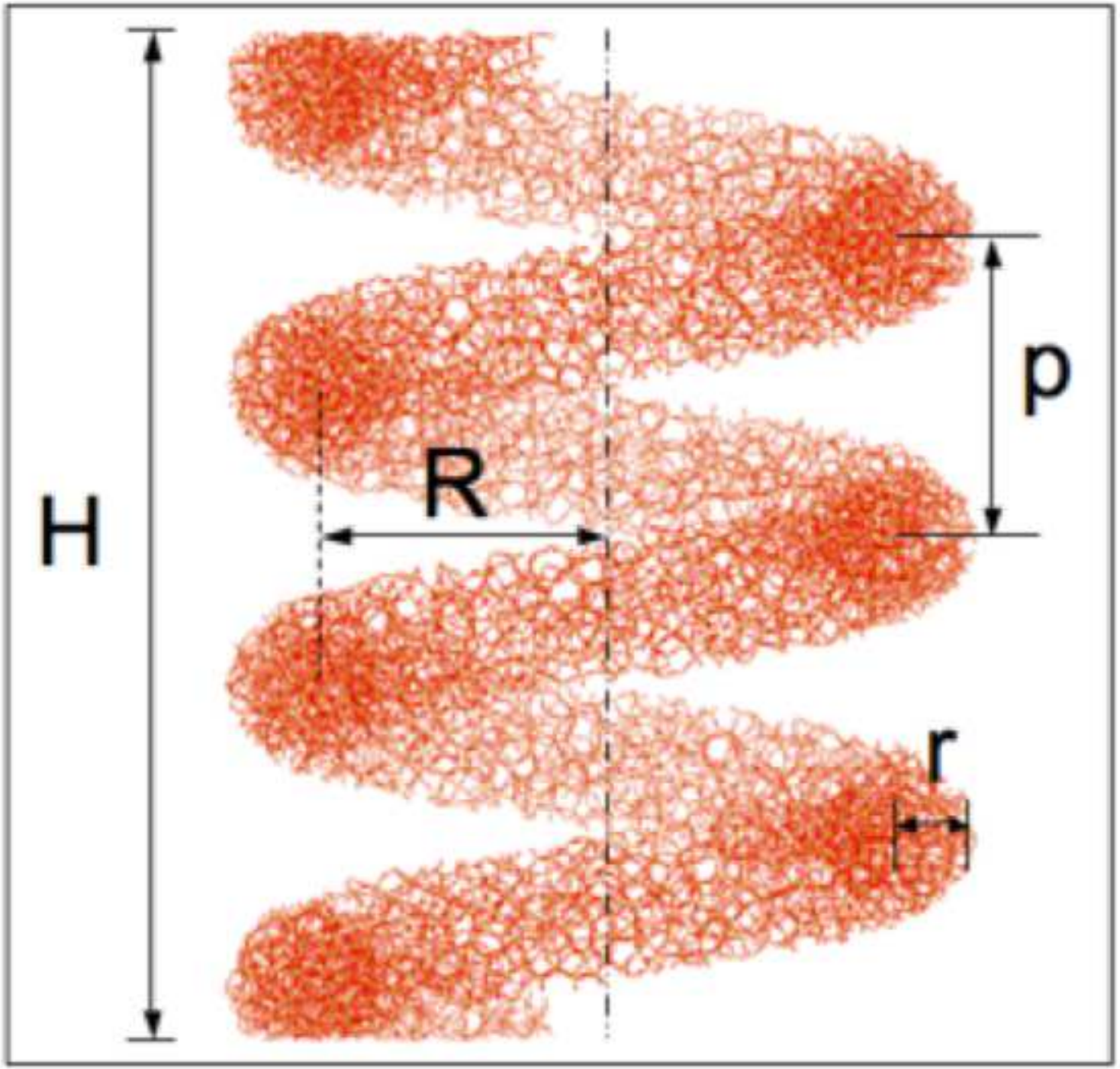

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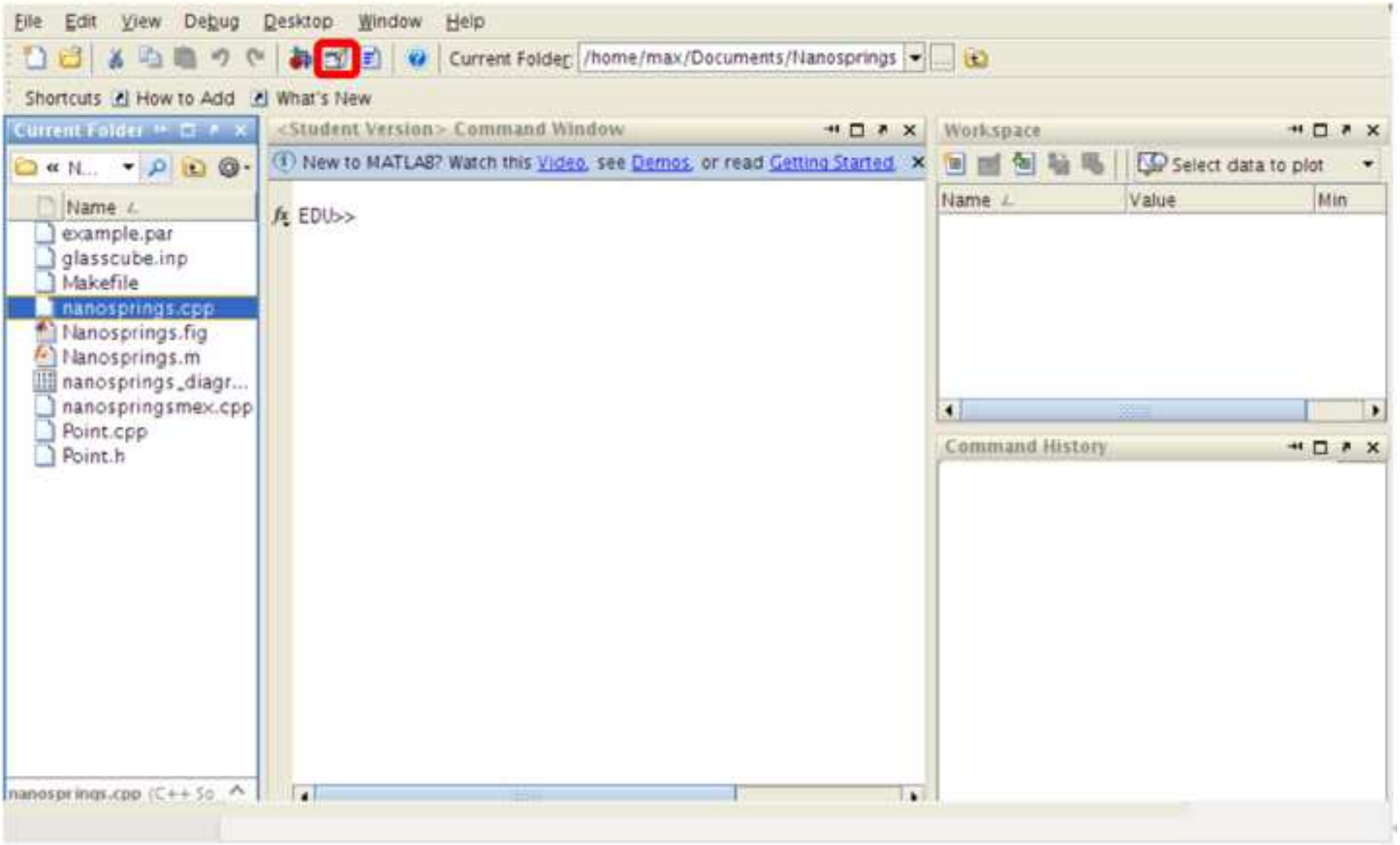

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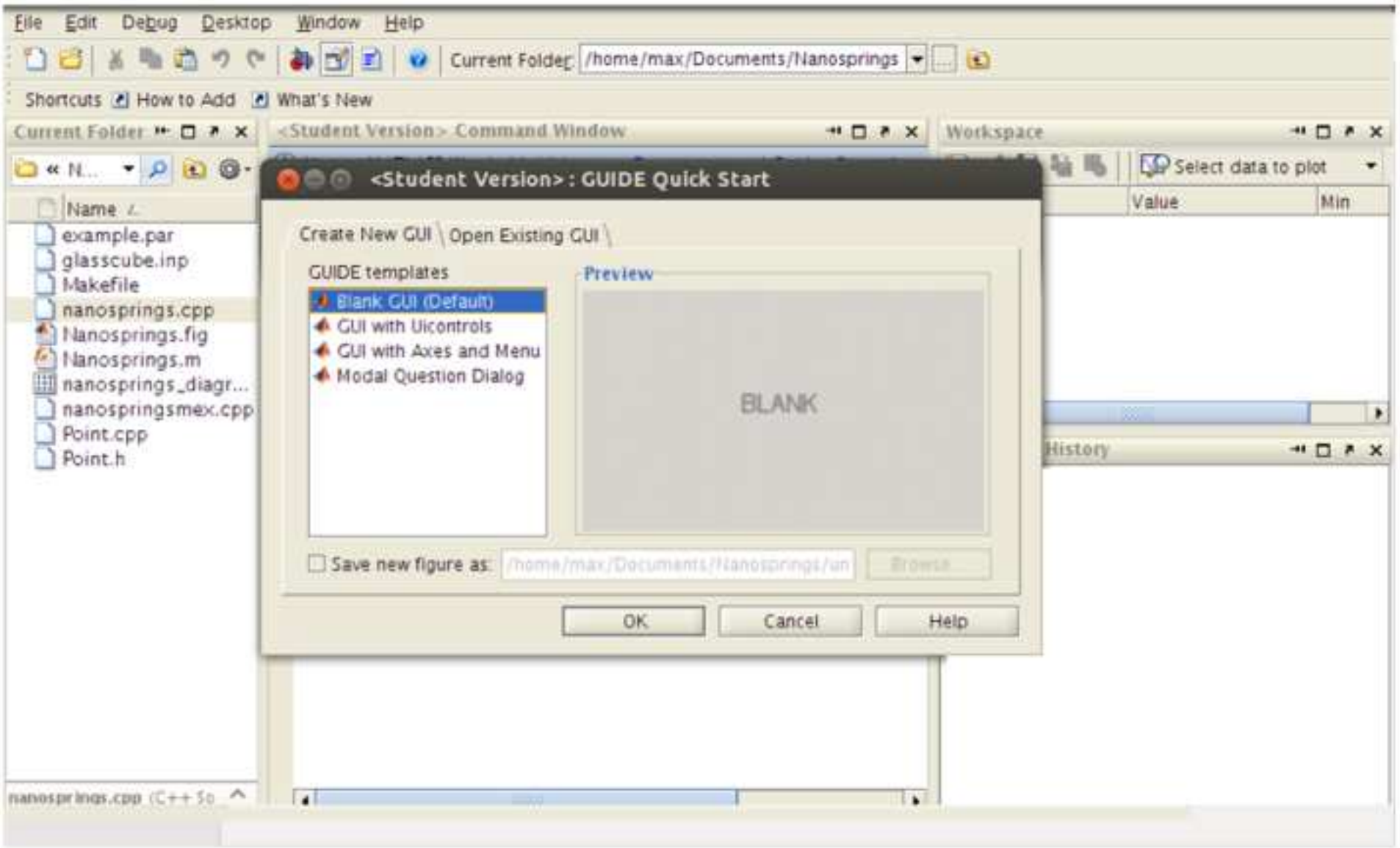

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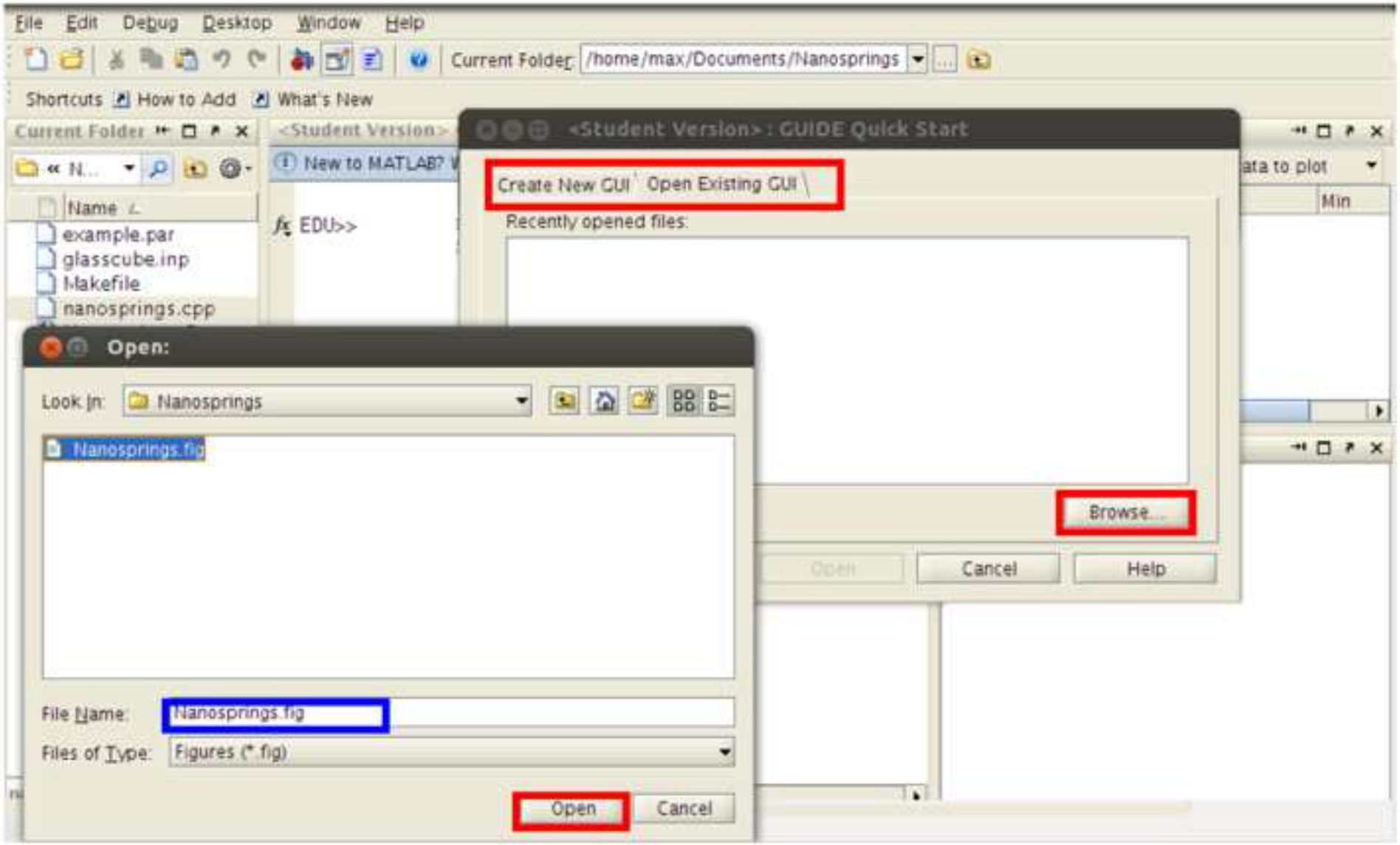

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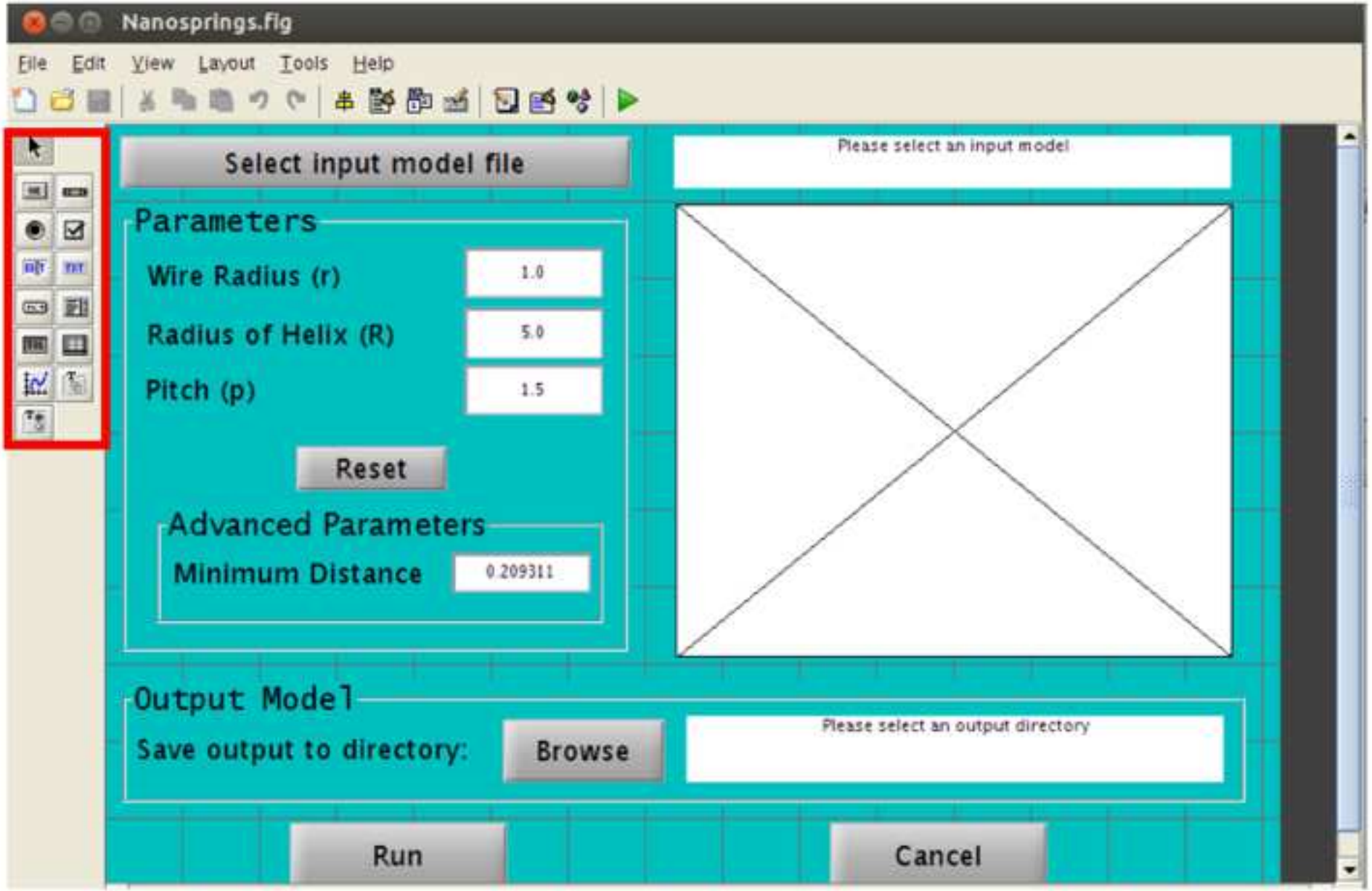

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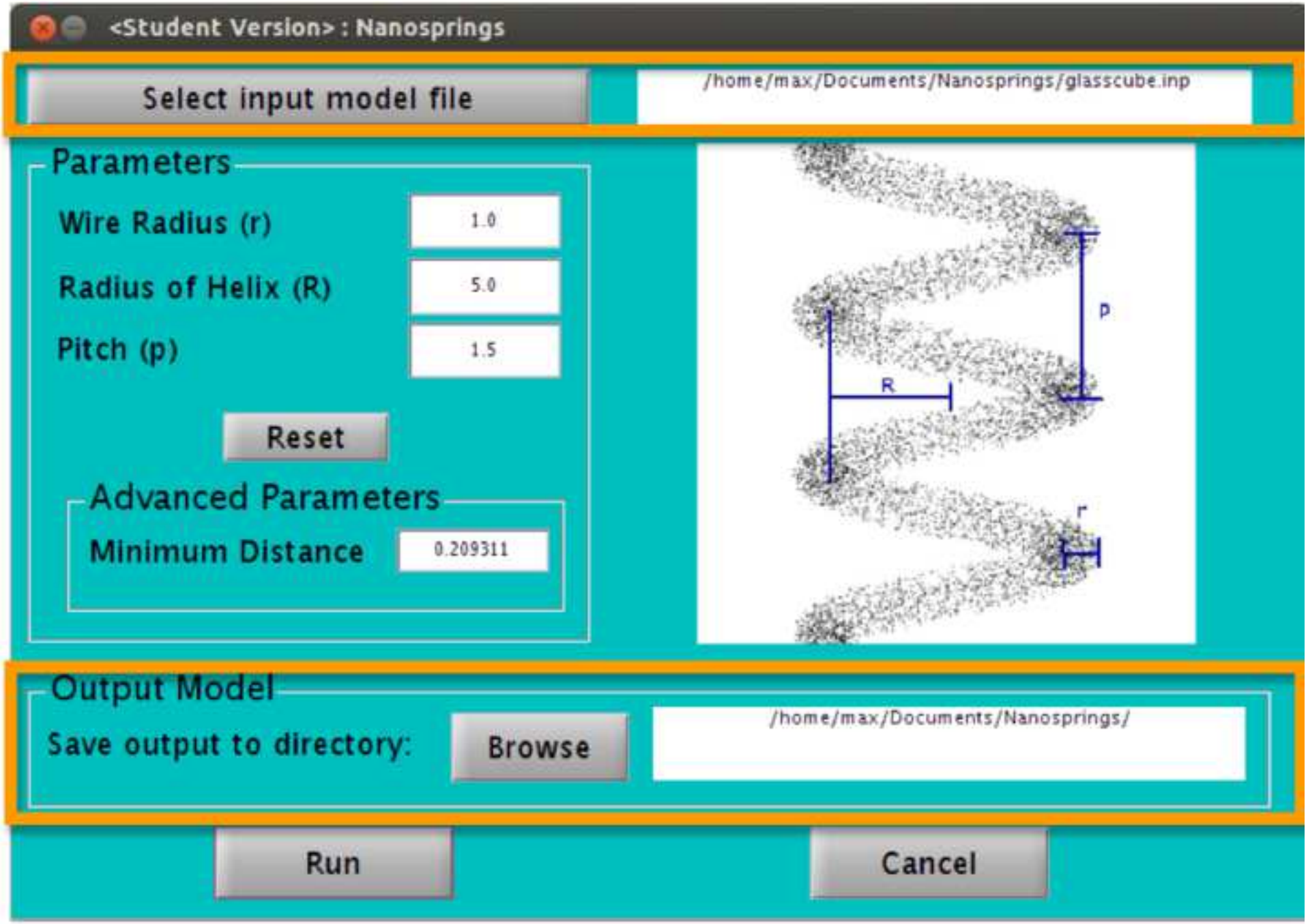

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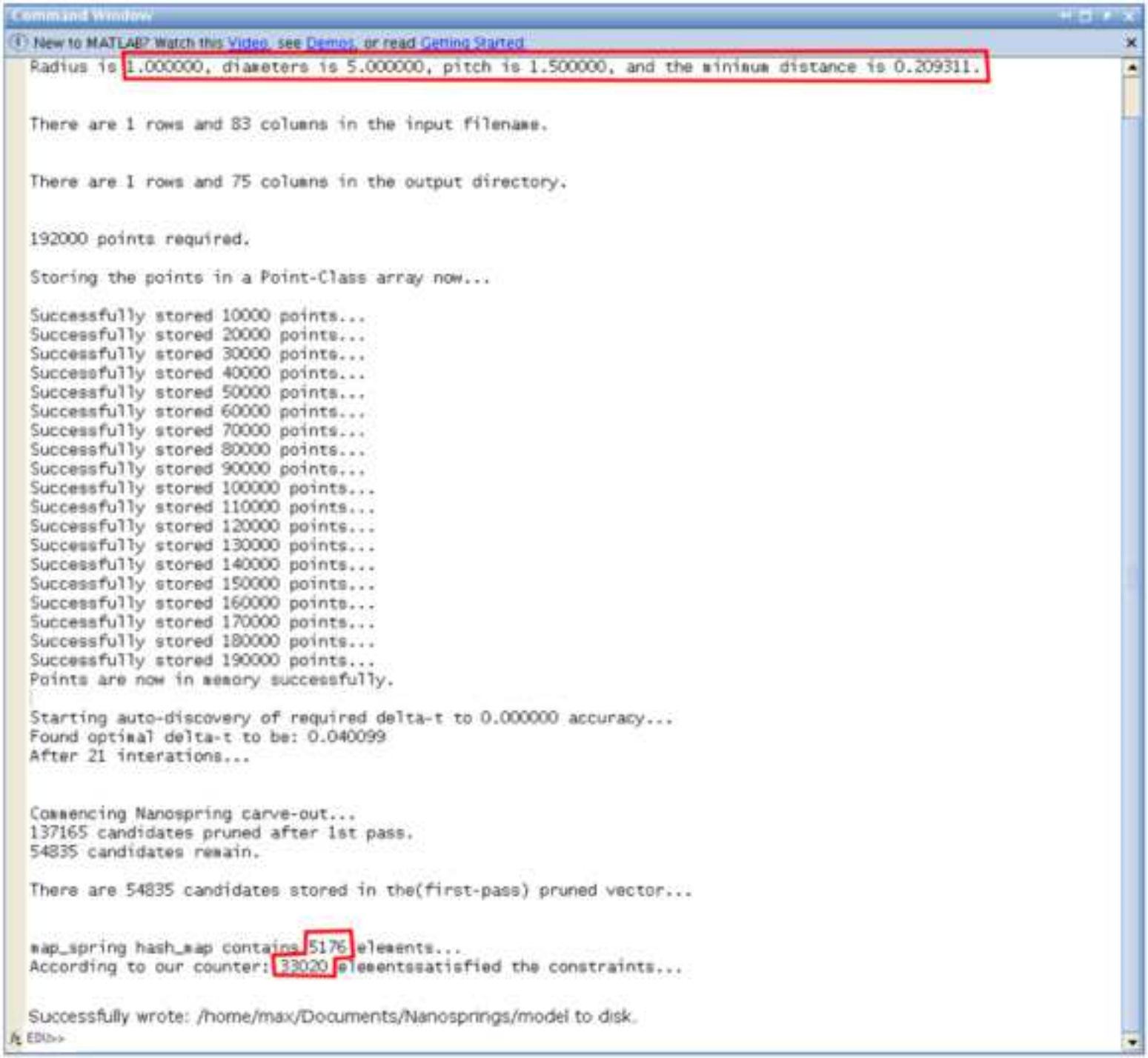

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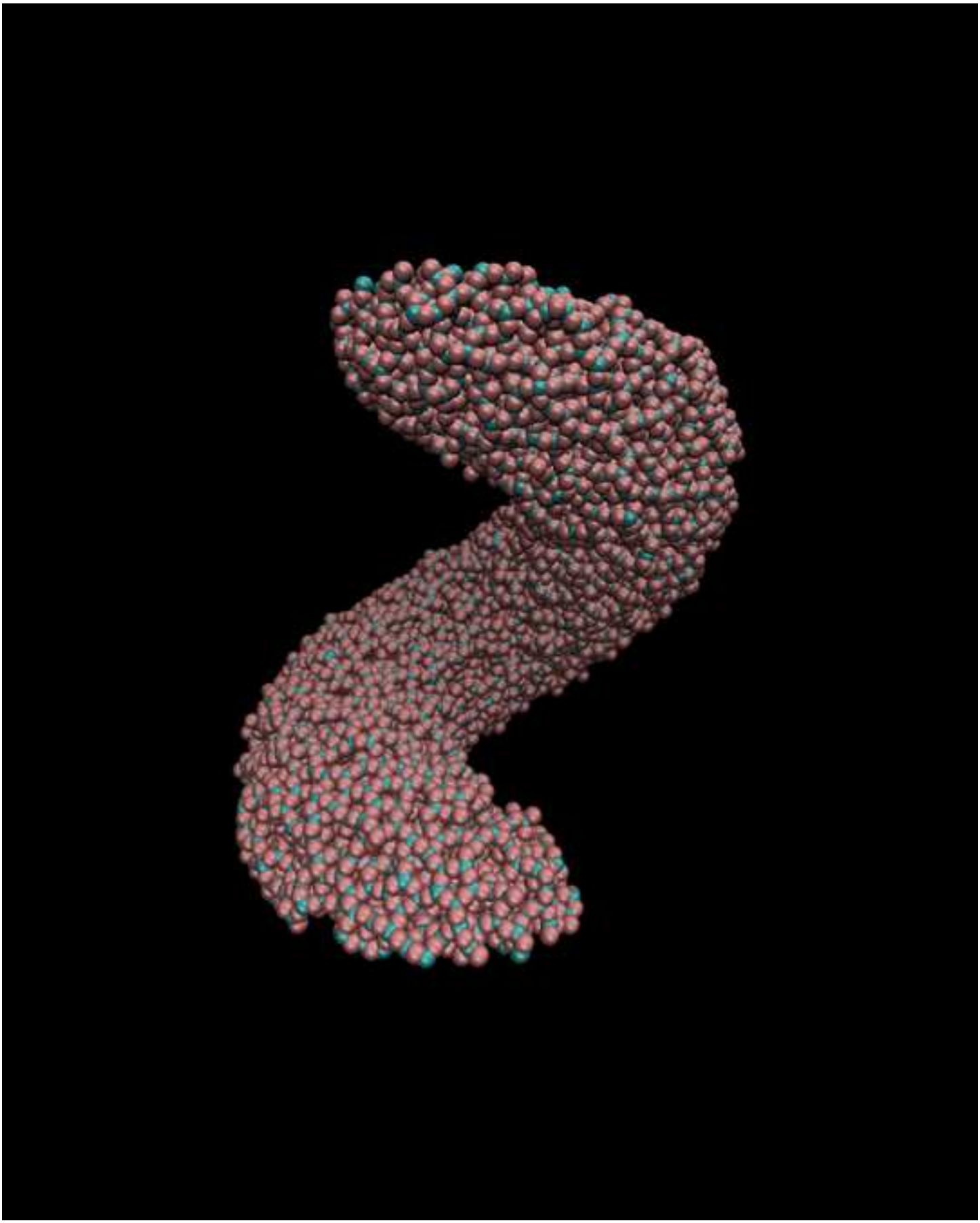

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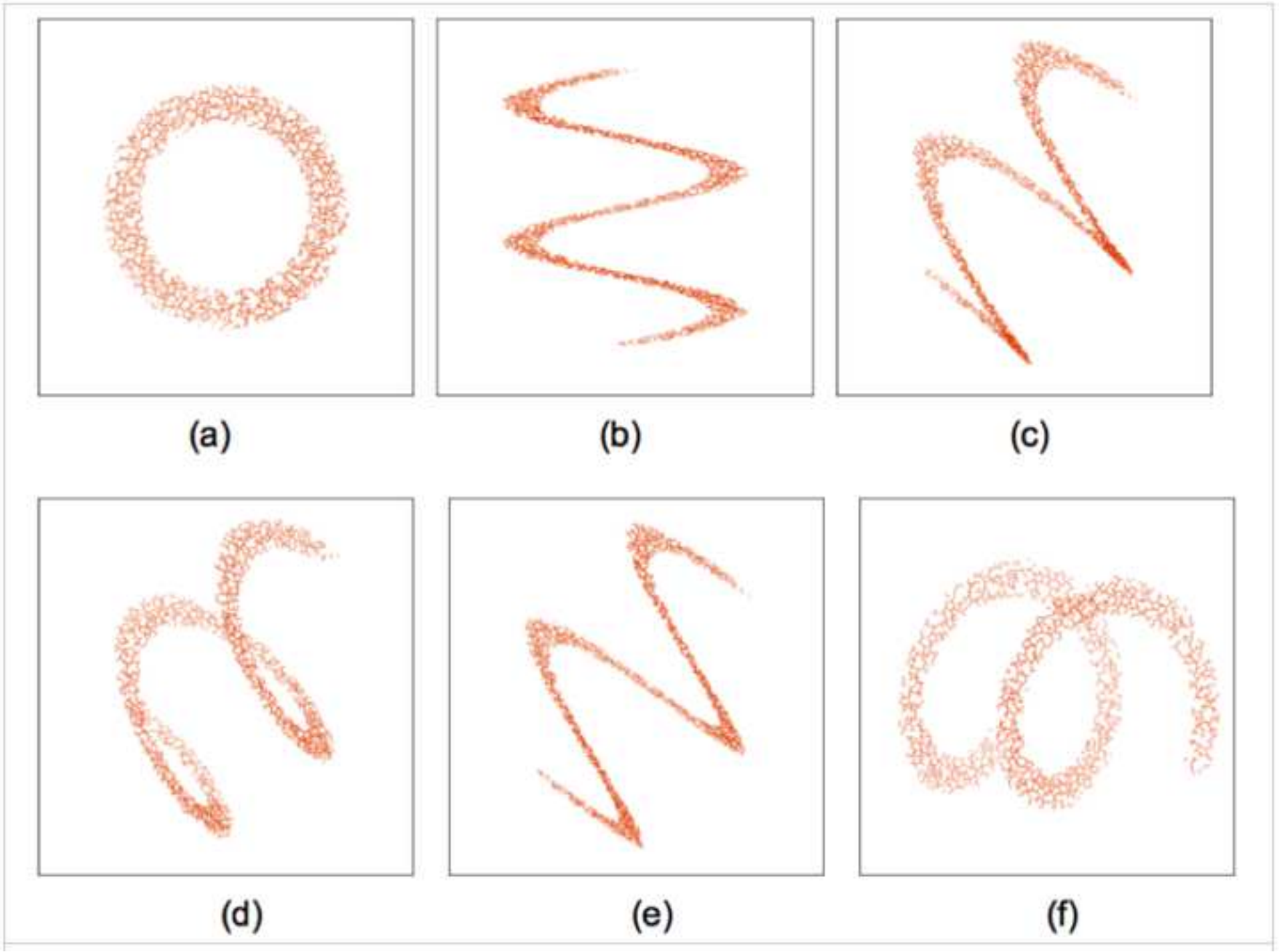

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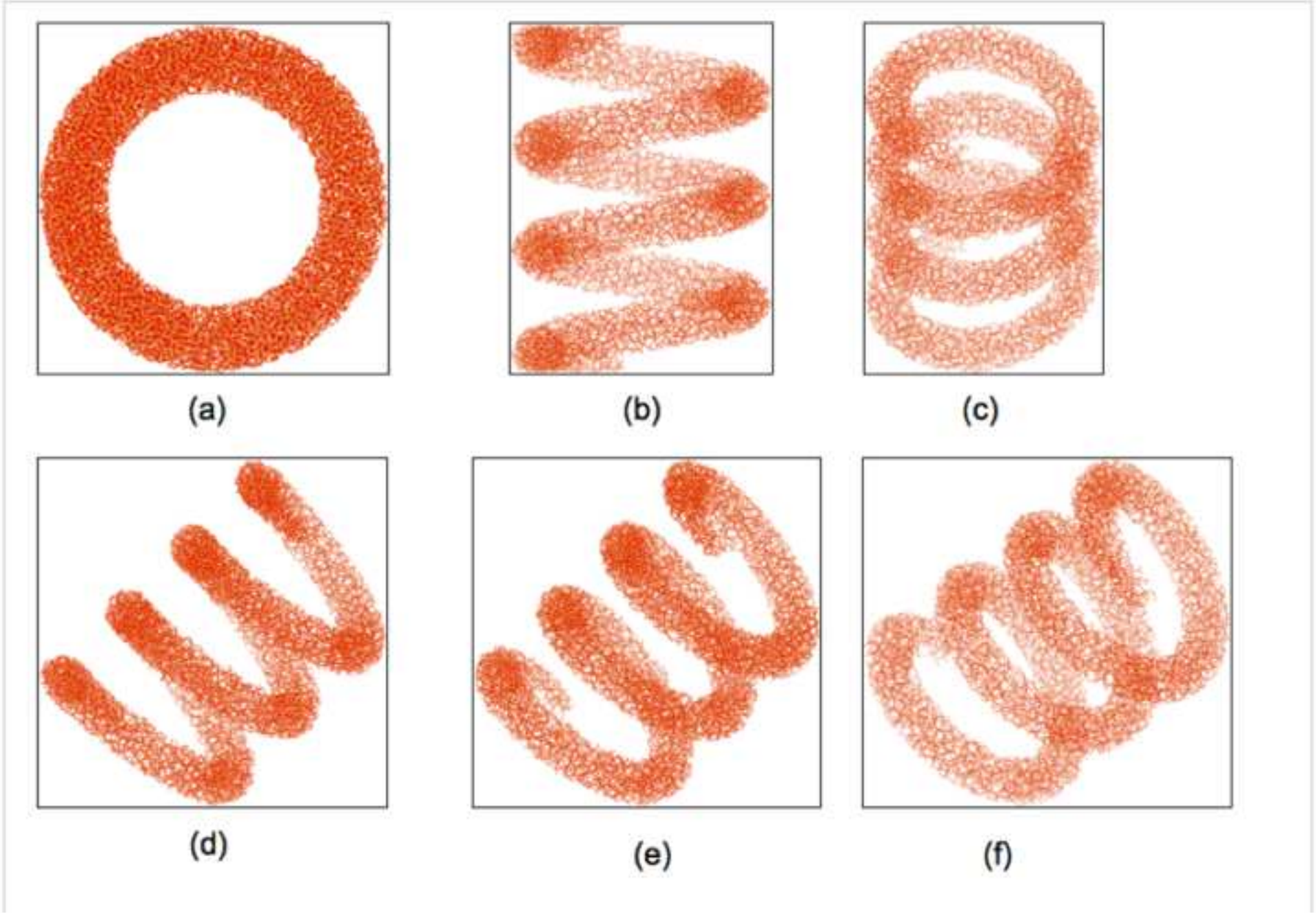

Excel Spreadsheet- Table of Materials/Equipment

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Name of Material/ Equipment	Company
MATLAB numerical computing software	Mathworks
NanospringCarver program code and files	UC Merced - open source
MATLAB GUI files	UC Merced - open source
Atomistic bulk glass input file	UC Merced - open source
IFrIT visualization software	Open source software
LAMMPS molecular dynamics software	Open source software

Catalog Number	Comments/Description
http://www.mathworks.com/products/matlab/description1.html [24]	See Protocol Introduction
http://tinyurl.com/qame8dj [26]	See Protocol Section 1 (Step 1.2)
http://tinyurl.com/qame8dj [26]	See Protocol Section 1 (Step 1.2)
http://tinyurl.com/qame8dj [26]	See Protocol Section 1 (Step 1.2)
http://sites.google.com/site/ifrithome/ [19]	See Protocol Section 3
http://www.lammps.sandia.gov/ [32]	See Protocol Section 4

Animated Figure1 (video and/or .ai figure files)

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April 8, 2014

Dear Editor:

Please find enclosed our manuscript JoVE51372 entitled "*Scalable Nanohelices for Predictive Studies and Enhanced 3D Visualization*," by Meagher, Doblack, Ramirez and Davila, which we submitted for your consideration to be published in the *Journal of Visualized Experiments (JoVE)*.

Below are our responses to each of the **Editorial comments** provided via email on February 24, 2014.

(1) Your editor made some minor copy edits and changes to formatting in your manuscript. Additionally all of the edits you made to the manuscript have been incorporated. Please use the most current version as you move forward with your revisions. You can find the updated manuscript under "file inventory" and download the microsoft word document.

Response: We have used the most current version of our manuscript (available under "file inventory") for our revision and kept previous overall changes and format in mind. We have submitted this revised version and changed the text color to purple to identify all of our manuscript edits.

(2) Thank you for providing detailed screen shots to guide the script-writer. These were included as a separate document and were not sent to peer review. Additionally they will not be published.

Response: We have kept a few of the screen shots in this revised version as they are deemed useful since the manuscript refers to them explicitly, to maintain the clarity of the work in the manuscript. We have added a note in green regarding figure numbers in the Table and Figure Legends section for clarification.
Question1: Would all screen shots be included in the video session or is the video crew intending to take close-up shots that attempt to be as clear and explicit?

(3) Some of your introductory material was out of the scope of a JoVE manuscript. This text was moved to a supplemental document (with two supplemental figures) and will be available with your manuscript at publication.

Response: This is fine. The material shifted to "Supplemental Material" does not affect the clarity of the rest of the manuscript. We have revised slightly the text however as shown in green in section entitled "[Supplemental Material]" at the end of this revised version.

(4) The figure legends were removed from the [insert here] references and will be added with the figures at integration.

Response: This is fine. No further adjustments were required in the revised version. We have also revised Table 1 to reflect appropriate references and uploaded to the JoVE website.
Question2: Regarding Figure 8 and Animated Fig1, how would the Animated Fig1 be accessed by a reader of the manuscript? Currently, the related statement states "supplement" and it is not clear what this means exactly.

(5) Please expand your discussion section to focus more on the details of the protocol and cover the following in detail and in paragraph form: 1) modifications and troubleshooting, 2) limitations of the technique, 3) significance with respect to existing methods, 4) future applications and 5) critical steps within the protocol.

Response: We have expanded the topics suggested in the discussion section.

(6) Please make sure that your references comply with JoVE instructions for authors- your manuscript will not pass internal review unless the reference formatting is correct. In-text formatting: corresponding reference numbers should appear as superscripts after the appropriate statement(s) in the text of the manuscript. Citation formatting should appear as follows: (For 6 authors or less list all authors. For more than 6 authors, list only the first author then *et al.*): [Lastname, F.I., LastName, F.I., LastName, F.I.

Article Title. *Source*. **Volume** (issue), FirstPage – LastPage, DOI, (YEAR).] JoVE follows recommended formatting for release to PubMedCentral, for specific reference questions please see the following: http://www.ncbi.nlm.nih.gov/staff/beck/citations/citationtags.html

Response: We have ensured that our references comply with JoVE instructions provided to authors.

(7) Please keep the editorial comments from your previous revisions in mind as you revise your manuscript to address peer review comments. For instance, if formatting or other changes were made, commercial language was removed, etc., please maintain these overall manuscript changes.

Response: We have kept previous editorial comments, overall changes and format in mind.

(8) Please take this opportunity to thoroughly proofread your manuscript to ensure that there are no spelling or grammar issues. Your JoVE editor will not copy-edit your manuscript and any errors in your submitted revision may be present in the published version.

Response: We have thoroughly proofread this revised version, and found no spelling or grammar issues.

Below are our responses to each of the **Reviewer's comments** provided via email on February 24, 2014.

Reviewer #1: "This article is of significant importance to the modeling of an important new class of advanced materials. The article clearly and concisely describes two methodologies that show promise. It should be most helpful to a growing community of researchers."

Response: Thank you for taking the time to review our manuscript and for your comments and encouraging words.

Reviewer #2: "Is the rationale and background for the technique adequately explained? When appropriate, does the author discuss limitations and mention alternative approaches? - The introduction explains the rationale and background for the approach presented. However, the authors need to discuss and compare alternatives to their approaches."

Response: Thank you for taking the time to review our manuscript and for your comments and suggestions. We have expanded the Introduction section further to discuss alternatives to our approaches.

Reviewer #2: "Minor concerns:
- A flowchart would be helpful for describing the process
- Alternative approaches should be discussed either in the Introduction or the Discussion section
- Quantify "accurate" throughout the Discussion section.
- Provide examples of "artifacts" that were not detected.
- Why is this approach more scaleable than others?"

Response: Below are our individual comments to the above items
-Although a flowchart might help to visualize this work, there is not one available that offers an advantage over the provided text, protocol and figures.
-We have expanded the Introduction section further to discuss alternatives to our approaches.
-We have revised this term and/or clarified accordingly throughout the Discussion section.
-We have expanded the description of the "artifacts" detected upon visual inspection.
-We have expanded the description of "scalable" in the manuscript. The intension was to convey the idea that the size of the model and spring parameters could be easily altered.

Reviewer #3: "There are a couple of points that are not clear in the description. On one hand the authors mention several times that this method produces "realistic models". What do they mean by this?. What

makes it a realistic model?. What type of parameters can they compare to experiments to determine that it is 'realistic'?."

Response: Thank you for taking the time to review our manuscript and for your comments and suggestions. The term "realistic models" was used once in the Abstract section as a general statement. The goal was to describe the need to develop representative helical models to study their atomic structure. No further adjustments were required on this point in the revised version.

Reviewer #3: "They also mention that in some simulations the model produces 'artifacts'. What type of artifacts?. This should be clarified so that people using the software can find out when an artifact has been produced."

Response: We have expanded the description of the "artifacts" detected upon visual inspection.

Reviewer #3: "Page 3, there is a sentence that ends as: "the open-source visualization software" which visualization software are they referring to?"

Response: The above sentence and reference [19] has been edited for clarity. No further edits are needed.

Reviewer #3: "A suggestion: maybe a short description on how to change the initial configuration file (glasscube.inp) to read other input files for different systems, would be useful for those people interested in systems other than silica.

Response: A brief description has been added as suggested to clearly describe this idea.

Finally, we have edited slightly the text and figure captions shifted to the "Supplemental Material" (changed the text color to purple as before to identify all necessary edits).

Please let me know if you have any questions or concerns about this latest submission. I am available to talk by phone or Skype at your earliest convenience any weekday (except for Tuesdays) for efficiency.

We hope that you find our paper interesting and worth publishing in the JoVE journal. We look forward to hearing from you soon. Thank you for your time and consideration.

Sincerely,

Lilian P. Dávila, Ph.D., Assistant Professor
Materials Science and Engineering, University of California, Merced
e-mail: ldavila@ucmerced.edu, Phone: (209) 228-4707

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