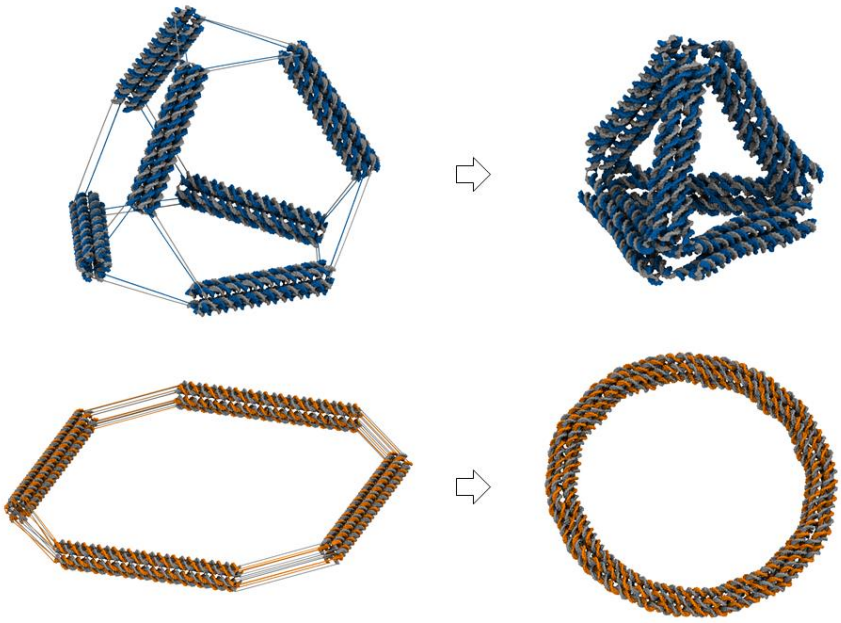
SNUPI (Structured NUcleic acids Programming Interface)

1. Release note

○ **v2.00**

- Wireframe and topologically-closed circular design can be analyzed directly from caDNAno input files (Example 4).
- Analysis results can be exported in the oxDNA input file format (Example 5).
- The model for the single-stranded DNA part is improved.



Wireframe (tetrahedron) and closed (ring-shaped) structures

2. System requirement

○ The implementation of SNUPI was targeted at the personal computer.

○ The pretested computing environment

- Windows 10, 64 bit (Graphical user interface was tested in 1920×1080 resolution)
- MacOS version 10.9.5, 64 bit
- CentOS Linux 7.2.1511, 64 bit

○ SNUPI was compiled using the Standalone Application Compiler in MATLAB.

○ MATLAB Runtime version R2019a (9.6) for the operating system should be installed.

- Installer site: http://www.mathworks.com/products/compiler/mcr/index.html
- If the runtime version is different, it may not run properly. Please check the version.

○ For Mac and Linux, SNUPI should run through command-input (See Example 3).

3. Preparation for the structural analysis

○ Download the SNUPI file.

- SNUPI site: https://github.com/SSDL-SNU/SNUPI

○ The following files are included.

• SNUPI_GUI.exe	SNUPI with a graphical user interface.
• EXAMPLE\<Ex_files>	Example design files.
• FILES\snupi.exe	Solver file.
• FILES\Default.snp	Default analysis options file.
• FILES\Input.txt	The temporary location of an input design.
• INPUT\<input_files>	Input files will be temporarily located in this folder.
• OUTPUT\<output_files>	Output files will be located in this folder.

○ The caDNAno program should be installed to prepare or modify design files.

- caDNAno site: https://cadnano.org/

○ Notes on design.

- The scaffold strand should be not circular but linear to generate a pdb file.
- BP-deletion should not be placed on the BPs of crossover and nick.
- The double-strand break is not considered in the analysis.

○ The installation of the VMD program is recommended to visualize the results.

- VMD site: https://www.ks.uiuc.edu/Research/vmd/

4. General procedure

● Step 1. Run SNUPI.

● Step 2. Select a design file: Design file (.json) should be assigned but sequence file (.csv) is optional.

● Step 3. Select the options (.snp).

● Step 4. Perform the analysis: Result files are saved in the OUTPUT folder.

● Step 5. Post-process the results.

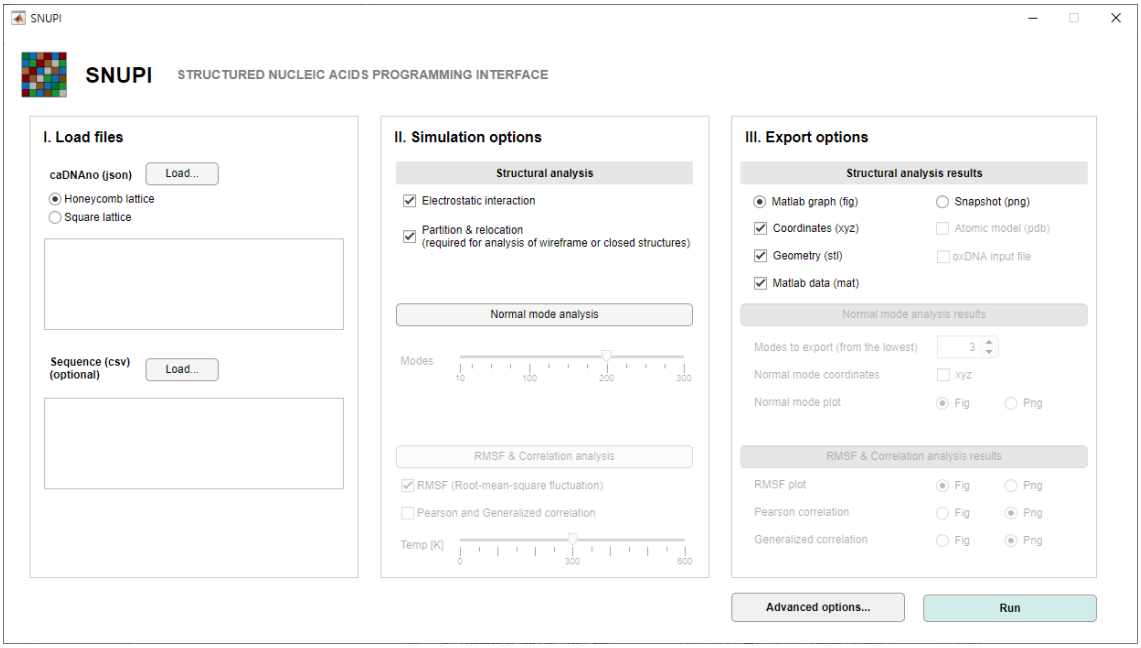
5. Examples

Example 1: Simple structural analysis using the default option.

○ This example describes how to analyze a design file using the default option.

● Step 1. Run SNUPI.

• Execute 'SNUPI_GUI.exe.'



SNUPI graphical user interface (GUI) window.

• Description of the GUI window.

[I. Load files]

- caDNAno (json): select a design file and its lattice type.
- Sequence (csv): select the corresponding sequence file (optional).

[II. Simulation options]

- Structural analysis: select if applying electrostatic interaction.
- Normal mode analysis: select (1) whether performing the analysis and (2) the lowest mode number to calculate.
- RMSF & Correlation analysis: select (1) whether performing the analysis and (2) temperature.

[III. Export options]

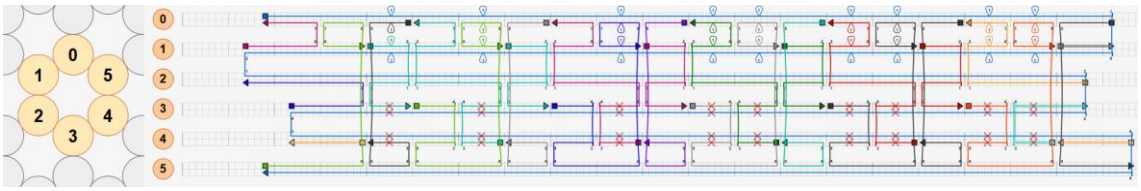
- Structural analysis results: select the exporting file type of the final configuration.
- Normal mode analysis results: select (1) the modes to export, (2) whether exporting 'xyz' files and (3) plot type of each mode shape.
- RMSF & Correlation analysis results: select the plot type of (1) RMSF, (2) Pearson correlation, and (3) Generalized correlation.

● Step 2. Select a design file.

• Load the design file (EXAMPLE\Ex_6HB.json),

• Specify the 'Honeycomb lattice.'

• Sequence file (.csv) is not necessary.



Example design (Ex_6HB).

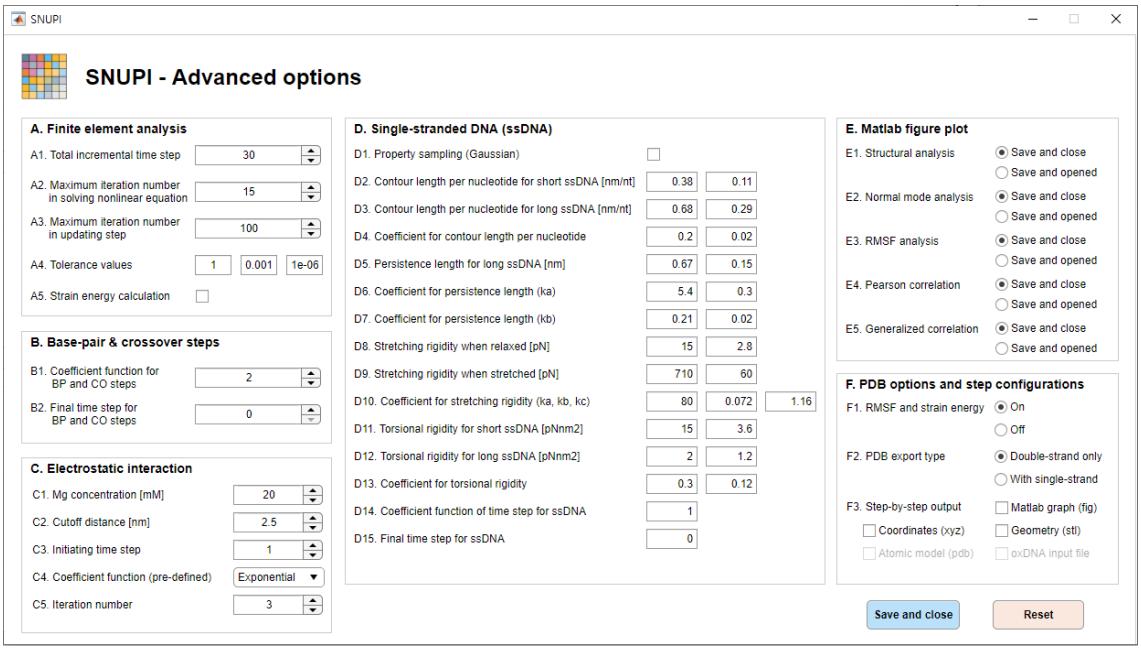
● Step 3. Select options.

• To use the default options, any modification in GUI is not necessary.

• In' Advanced options...', the values used in the analysis can be modified in more detail.

• Advanced options are described in the independent section (*SNUPI options*).

• To use the default options, press the 'Save and Close' button.



Advanced options window.

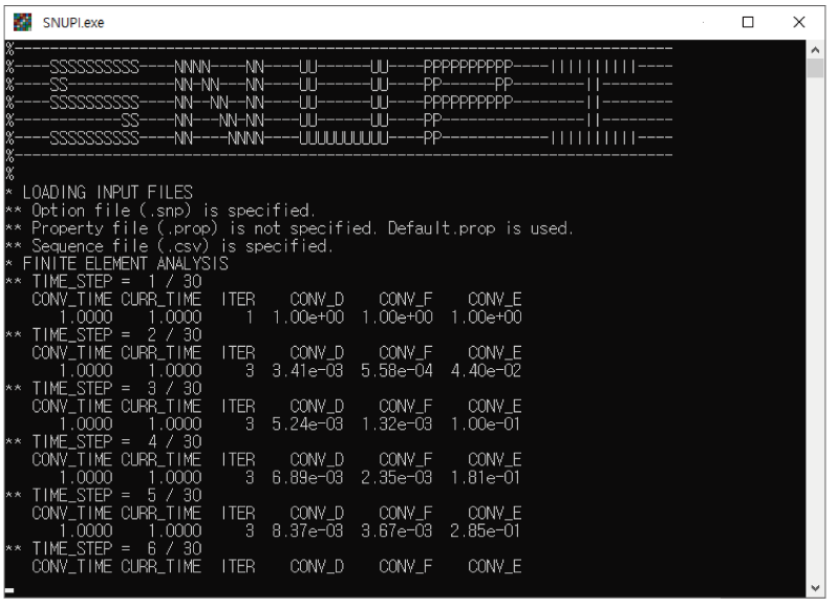
● Step 4. Perform analysis.

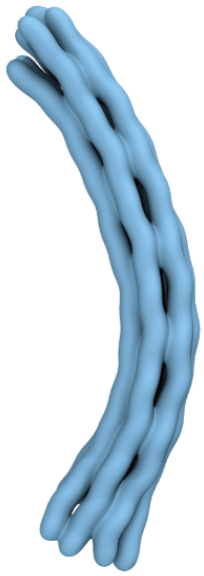
• Press the 'Run' button.

- The selected option (.snp) and design (.json) files are saved in the 'INPUT' folder.

- The analysis procedure is displayed in the command prompts as below.

- The log file is saved as an 'Ex_6HB.log' file in the 'OUTPUT' folder.





Analysis procedure and the predicted shape.

● Step 5: Post-process the results

• The output files are saved in the directory, 'OUTPUT\Ex_6HB_<time>'.

- The design file is saved as the 'Ex_6HB.json' file.
- Since the sequence file (csv) is not specified, mean properties are used.

• The employed options for the analysis were saved as 'OUTPUT\Ex_6HB.snp'.

- Since any option is not modified, the default options are used.
- The default file is provided as 'DEFAULT\Default.snp'.

• The final shape is saved as 'Ex_6HB_FINAL.fig', 'Ex_6HB_FINAL.xyz', 'Ex_6HB_FINAL.stl' files.

• The 'Ex_6HB.xyz' file can be rendered using the VMD program with the graphical options as above.

- Material: AOChalky
- Drawing Methods: QuickSurf
- Radius Scale: 3.8
- Renderer: Tachyon

• Results are saved in the 'Ex_6HB.mat' file (MATLAB).

- FE_DATA: Structural element connectivity (E_CONN)
  Global mass matrix (M_G)
- NLA_DATA: Initial nodal configuration for each incremental time step (INIT_NODE)
  Final nodal configuration for each incremental time step (FINL_NODE)
  Initial element triads for each incremental time step (INIT_TR)
  Final element triads for each incremental time step (FINL_TR)
  Global stiffness matrix for each incremental time step (K_G)
- NA_HELIX: Helix data
- NA_CROSS: Crossover data
- The unit of values is [pN] or [nm].

Example 2: Prediction of structural and dynamic properties.

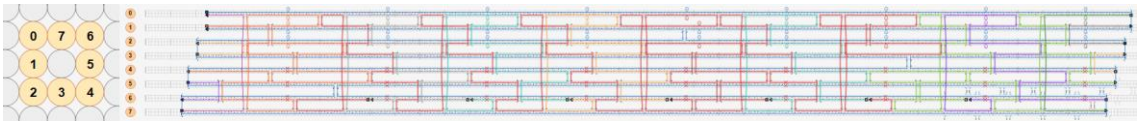
○ This example describes how to predict structural shape, mode shapes, and dynamic properties.

● Step 1. Run SNUPI.

- Execute 'SNUPI_GUI.exe.'

● Step 2. Select a design file.

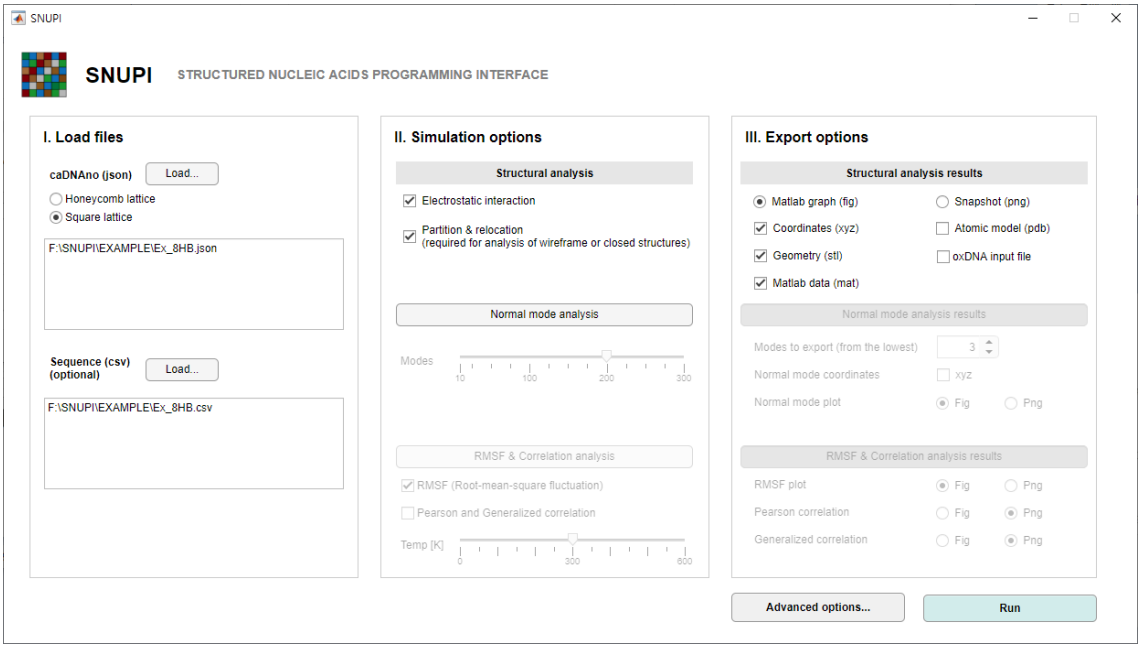
- Load the design file (EXAMPLE\Ex_8HB.json),
- Specify the 'Square lattice.'
- Load sequence file (EXAMPLE\Ex_8HB.csv).



Example design (Ex_8HB).

● Step 3. Select options.

- To export atomic representation, select the 'atomic model (.pdb).'
- To perform the normal mode analysis, select 'Normal mode analysis.'
  - The number of the lowest normal modes to calculate was set to 200 in default.
  - The number of the lowest normal modes to export was set to 3 in default.
- To additionally export 'xyz' files for mode shapes, select 'Normal mode coordinates.'
- To calculate dynamic properties, select 'RMSF & Correlation analysis.'
  - The root-mean-square fluctuation (RMSF) and correlation coefficients are calculated.
  - The default absolute temperature was set to 300 K in default.



SNUPI graphical user interface window.

● Step 4. Perform analysis.

• Press the 'Run' button.

- The selected option (.snp) and design (.json) files are saved in the 'INPUT' folder.
- The analysis procedure is displayed in the command prompts as below.
- The log file is saved as the 'Ex_8HB.log' file in the 'OUTPUT' folder.

● Step 5: Post-process the results

• The output files are saved in the directory, 'OUTPUT\Ex_8HB_<time>'.

- The design file is saved as the 'Ex_8HB.json' file.
- The sequence file is saved as the 'Ex_8HB.csv' file.
- Since the sequence file (.csv) is specified, sequence-dependent properties are used.

• The selected options for the analysis were saved as 'OUTPUT\Ex_8HB.snp'.

• The final shape is saved as files with different formats (.fig, .xyz, .stl, and .pdb).

• The 'Ex_8HB.pdb' file can be rendered using the VMD program with the graphical options as below.

- The topology file (.psf in VMD) should be first generated.
- Material: AOChalky
- Drawing Methods: NewCartoon
- Renderer: Tachyon

Predicted structural shape.

• Results of the structural analysis were saved in 'Ex_8HB.mat' file (MATLAB)

- FE_DATA: Structural element connectivity (E_CONN)
  Mass matrix (M_G)
  Total strain energy (TOTAL_SE)
- NLA_DATA: Initial nodal configuration for each incremental time step (INIT_NODE)
  Final nodal configuration for each incremental time step (FINL_NODE)
  Initial element triads for each incremental time step (INIT_TR)
  Final element triads for each incremental time step (FINL_TR)
  Stiffness matrix for each incremental time step (K_G)
- The unit of values is [pN] or [nm].

• The total strain energy values were saved in the Beta column of the 'Ex_8HB.pdb' file.

- The values are normalized in the range of 0 to 1.

• The total strain energy map in the 'Ex_8HB.pdb' file can be rendered using the VMD program below.

- Material: AOChalky
- Coloring Methods: Beta
- Drawing Methods: QuickSurf
- Renderer: Tachyon
- Color: Low strain energy (white), High strain energy (blue)

The total strain energy map.

• By performing the normal mode analysis, the eigensolutions were saved in the 'Ex_8HB.mat' file.

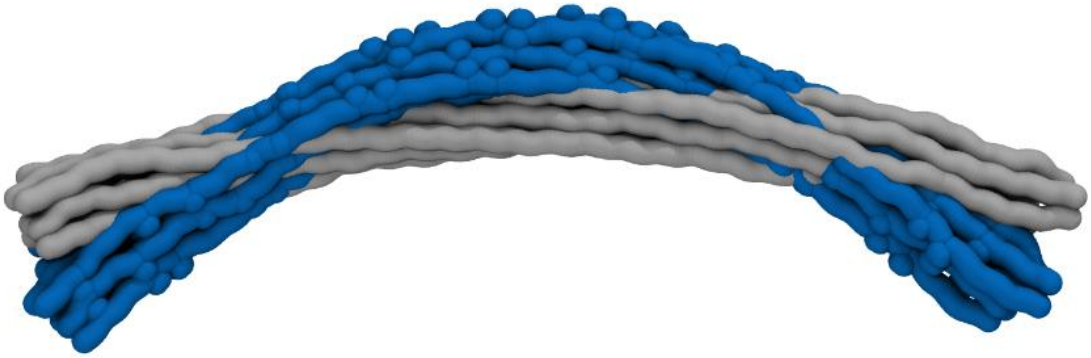
- NMA_DATA: Eigenvalues (EIG_VAL)
  Eigenvectors (EIG_VEC)

• The bending mode shape is obtained as the lowest (first) mode.

- The reference (final) shape is saved as 'Ex_8HB_MODE_0_REF.xyz' or 'fig' files.
- The k^{th} mode shape is saved as 'Ex_8HB_MODE_k.xyz' or 'fig' files.

• The 'xyz' files of mode shapes can be rendered using the VMD program with the graphical options as below.

- Material: AOChalky
- Drawing Method: Beads
- Color: Reference shape (gray), the lowest mode shape (blue)



The lowest mode shape.

• The dynamic properties were saved in the 'Ex_8HB.mat' file.

- NMA_DATA: RMSF values (RMSF)
  Pearson correlation coefficient (CORR_P_MAT)
  Generalized correlation coefficient (CORR_G_MAT)

• The RMSF values were saved in the Occupancy column of the 'Ex_8HB.pdb' file.

- The values are normalized in the range of 0 to 1.

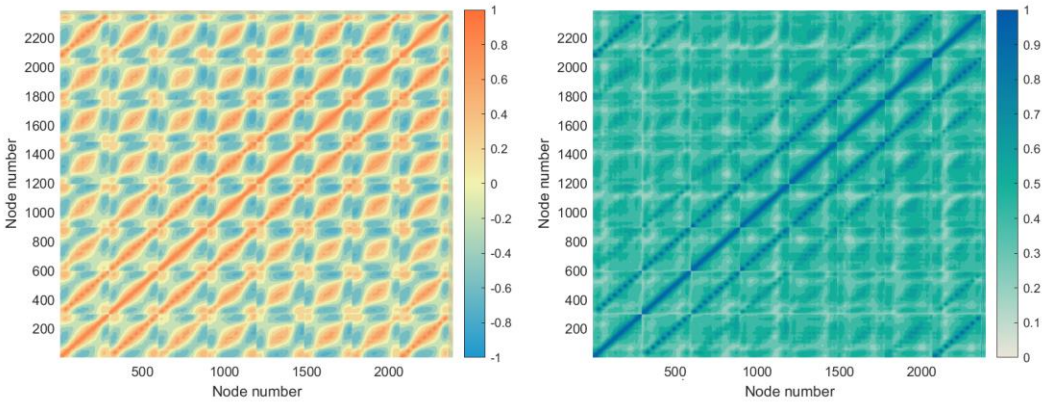
• The RMSF map in the 'Ex_8HB.pdb' file can be rendered using the VMD program below.

- Material: AOChalky
- Coloring Methods: Occupancy
- Drawing Methods: QuickSurf
- Renderer: Tachyon
- Color: Low fluctuation (white), High fluctuation (red)

RMSF map of the structure.

• Correlation coefficients are saved in the 'Ex_8HB_CORR' files.

- Pearson correlation coefficient: 'Ex_8HB_CORR_P.png'
- Generalized correlation coefficient: 'Ex_8HB_CORR_G.png'



Pearson (left) and generalized (right) correlation coefficients.

Example 3: Running SNUPI serially by specifying multiple design and options files.

○ The GUI program (SNUPI_GUI.exe) is a tool for executing the main SNUPI program (FILES\SNUPI.exe) with specifying design files (.json, .csv) and options (.snp).

○ In detail, the GUI program takes design files to the input folder (INPUT) and modifies the input text file (FILES\Input.txt) to indicate the design and option files.

○ It is also possible to execute SNUPI serially with multiple design files and options without the GUI.

● Step 1. Prepare design files.

- For the analysis, design files of topology (.json), sequence (.csv, optional), and option (.snp, optional) should be prepared with same name.
- Three designs are used here as follows.
  - EXAMPLE\Ex_6HB_default (.json)
  - EXAMPLE\Ex_6HB_NoElec (.json, snp)
  - EXAMPLE\Ex_8HB_NMA (.json, .csv, .pdb)

● Step 2. Indicate the design files.

- Modify the input text file
  - FILES\Input.txt

```
% Column 1: Lattice type, Honeycomb (H) or Square (S)
% Column 2: Directory of design files
% '%' represents a comment line
H       ..\EXAMPLE\Ex_6HB_default
H       ..\EXAMPLE\Ex_6HB_NoElec
S       ..\EXAMPLE\Ex_8HB_NMA
```

● Step 3. Perform analysis.

- Execute SNUPI (FILES\SNUPI.exe).
- Results will be saved in the output folder (OUTPUT).

○ Notes for design files

- 'Ex_6HB_default' and 'Ex_6HB_NoElec' have the same topology (.json).
- For 'Ex_6HB_default' design, there is no option file (.snp), so the default snp file (FILES\Default.snp) is used for its analysis. A user can modify the default snp file, then input files without snp files will be analyzed using the modified default snp file.
- For the 'Ex_6HB_NoElec' design, its option was modified not to include the electrostatic interaction by setting the option as follows.
  - DO_ES 0
- For the 'Ex_8HB_NMA' design, its option was modified to perform the normal mode analysis as follows.
  - DO_NMA 1

○ Notes for running SNUPI in Mac or Linux OS

- In Mac or Linux OS, the GUI program is not supported.
- In Mac or Linux OS, use '/' instead of '\' when modifying input text files (FILES\Input.txt).
- In Mac or Linux OS, SNUPI can be run in the terminal as follows.

  ./run_SNUPI.sh <matlab_runtime_directory>
- (Mac OS) For example,

  ./run_SNUPI.sh /Applications/MATLAB/MATLAB_Runtime/v96
- (Linux OS) For example,

  ./run_SNUPI.sh /usr/local/MATLAB/MATLAB_Runtime/v96

Example 4: Structural analysis of wireframe and topologically-closed circular structures

○ This example demonstrates the application of SNUPI analysis to predict the free-form shape of wireframe and topologically-closed circular structures using the partition and relocation method.

● Step 1. Run SNUPI.

- Execute 'SNUPI_GUI.exe.'

● Step 2. Select a design file.

- Load the design file (EXAMPLE\Tetrahedron.json or EXAMPLE\Ex_6HB_Ring.json)
- Specify the 'Honeycomb lattice.'
- Load sequence file (Ex_Tetrahedron.csv or Ex_6HB_Ring.csv).

Example designs (Left: Ex_Tetrahedron, Right: Ex_6HB_Ring).

● Step 3. Select options.

- To execute the partition and relocation option, select 'Partition and relocation.' (default: on)

● Step 4. Perform analysis.

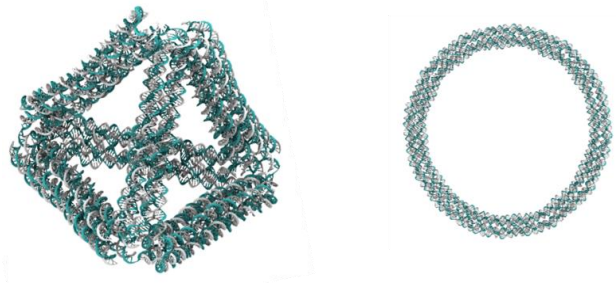
- Press the 'Run' button.
  - The selected option (.snp) and design (.json) files are saved in the ‘INPUT’ folder.
  - The analysis procedure is displayed in the command prompt as below.
  - The log file of the analysis procedure is saved in the 'OUTPUT' folder.
  - When the partition and relocation framework is applied without any issue, 'PARTITION & RELOCATION: DONE' is displayed in the command prompt and saved in the log file.

```
%-------------------------------------------------------------------------
%----SSSSSSSSSS----NNNN----NN----UU------UU----PPPPPPPPP----||||||||||----
%----SS----------NN-NN---NN----UU------UU----PP-------PP--------||--------
%----SSSSSSSSSS----NN--NN--NN----UU------UU----PPPPPPPPP---------||--------
%----------SS----NN---NN-NN----UU------UU----PP----------------||--------
%----SSSSSSSSSS----NN----NNNN----UUUUUUUUU----PP----------|||||||||----
%-------------------------------------------------------------------------
%
% VERSION: 2.00
%-------------------------------------------------------------------------
* INITIAL CONFIGURATION
  - INPUT FILE: EX_Tetrahedron
  - OPTIONS ASSIGNED (.snp)
  - SEQUENCE ASSIGNED (.csv)
  - PARTITION & RELOCATION: DONE
  - CPU TIME (INITIAL CONFIGURATION) = 31.77 [s]
%-------------------------------------------------------------------------
* STATIC FINITE ELEMENT ANALYSIS
* INPUT FILE: EX_Tetrahedron
* TIME_STEP =  1 / 30
  CONV_TIME CURR_TIME  ITER    CONV_D    CONV_F    CONV_E
     1.0000    1.0000     1  1.00e+00  1.00e+00  1.00e+00
* TIME_STEP =  2 / 30
  CONV_TIME CURR_TIME  ITER    CONV_D    CONV_F    CONV_E
     1.0000    1.0000     4  1.97e-03  8.42e-05  1.41e-02
* TIME_STEP =  3 / 30
  CONV_TIME CURR_TIME  ITER    CONV_D    CONV_F    CONV_E
     1.0000    1.0000     4  2.10e-03  9.82e-05  1.50e-02
```

Analysis procedure (Ex_Tetrahedron).

● Step 5. Post-process the results.

• The global configurations are predicted as below.



Prediction (Left: Ex_Tetrahedron, Right: Ex_6HB_Ring).

○ Reference of the designs

- Tetrahedron: Jun, Hyungmin, et al. "Automated sequence design of 3D polyhedral wireframe DNA origami with honeycomb edges." *ACS Nano* 13.2 (2019): 2083-2093.

- Ring: Lin, Chenxiang, et al. "Purification of DNA-origami nanostructures by rate-zonal centrifugation." *Nucleic Acids Research* 41.2 (2013): e40-e40.

Example 5: Outfile generation for oxDNA simulation

○ The coordinates (conf) and topology (top) can be generated for performing oxDNA simulation.

○ This example describes how to generate oxDNA inputs (conf and top files).

● Step 1. Run SNUPI.

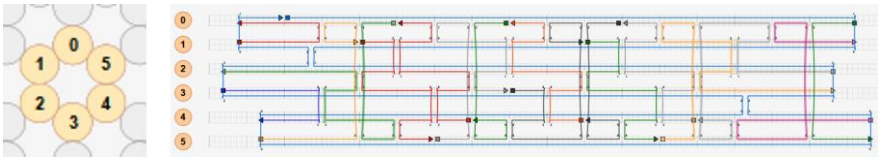
• Execute 'SNUPI_GUI.exe.'

● Step 2. Select a design file.

• Load the design file (Ex_6HB.json).

• Specify the 'Honeycomb lattice.'

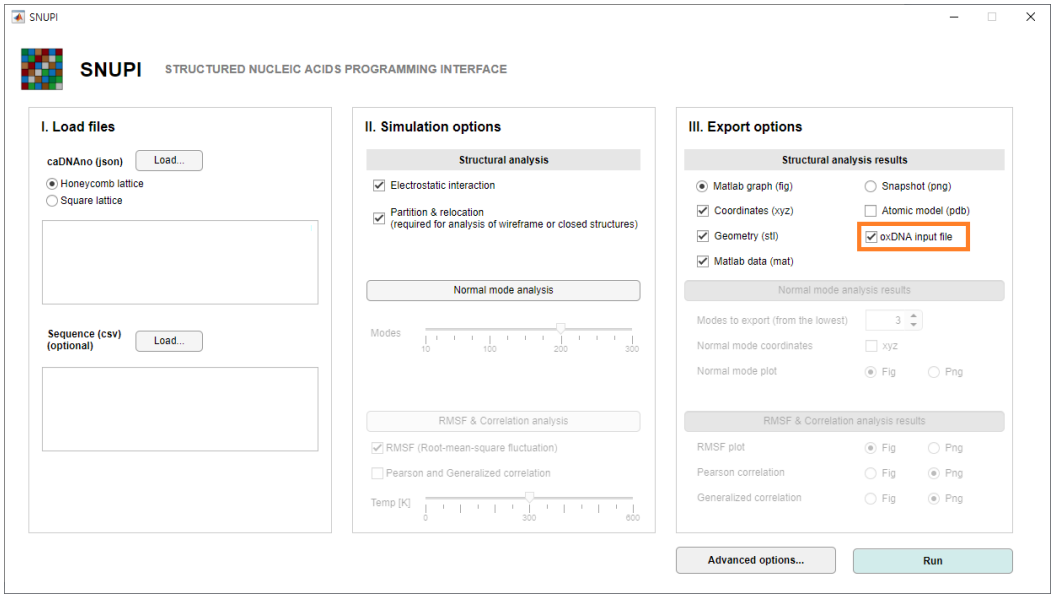
• Load sequence file (Ex_6HB.csv).



Example design (Ex_6HB).

● Step 3. Select options.

• To export oxDNA inputs, select the 'oxDNA input file.'



● Step 4. Perform analysis.

• Press the 'Run' button.

- The analysis procedure is displayed in the command prompt.

- The log file is saved as the 'Ex_6HB.log' file in the 'OUTPUT' folder.

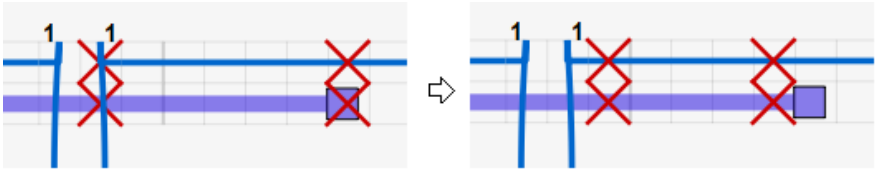
● Step 5: Post-process the results

• OxDNA input files (Ex_6HB.conf and Ex_6HB.top) are saved in the directory, 'OUTPUT\Ex_6HB_<time>'.

6. Troubleshooting

○ Design error #1

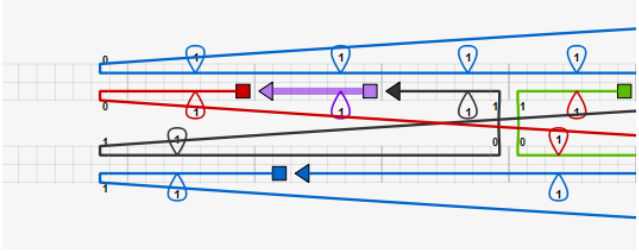
- An error could occur due to difficulty in defining a triad of base-pairs by the base-pair deletion.
- Please check that the design file has the base-pair deletion at the crossover or terminal end of strands.
- If so, move the location of the base-pair deletion to the neighboring.



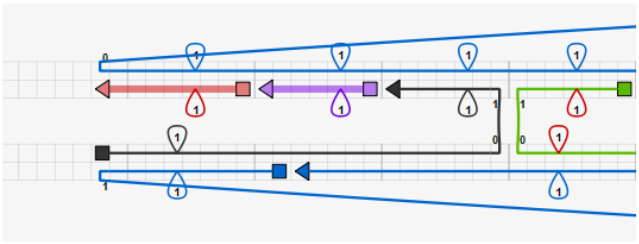
○ Design error #2 (closed design)

- The end-to-end connection should be on the regular helix

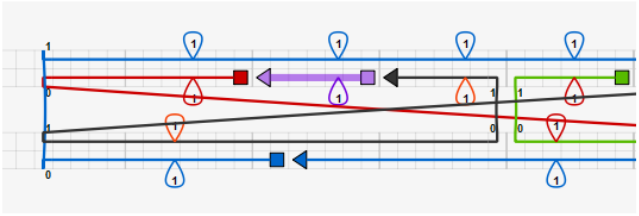
Regular base-pair connection (O)



Nicked base-pair connection (O)



Crossover connection (X)



7. Options

Finite element analysis

○ TIME_STEP

Total incremental time step (T).

This represents the total incremental time step for structural analysis. The larger the step is, the finer the properties change from the initial to the final structure. In general, the total step between 20 and 40 is appropriate.

This option corresponds to [A1] in the 'Advanced options' window.

Default: 30

○ ITER_NL_NUM

Maximum iteration number in solving equations in each incremental time step.

This represents the maximum iteration number for finding a solution in each incremental time step. If no solution is found in each step, the properties are adjusted.

This option corresponds to [A2] in the 'Advanced options' window.

Default: 15

○ ITER_TIME_NUM

Maximum iteration number in updating the incremental time step.

This represents the maximum number of adjustments of properties in each incremental time step.

This option corresponds to [A3] in the 'Advanced options' window.

Default: 100

○ TOL

Tolerance value for displacement, force, and energy criteria.

Two of the three tolerance values are generally specified lower than 1.

This option corresponds to [A4] in the 'Advanced options' window.

Default: 1 1E-3 1E-6

○ DO_SE_CAL

Strain energy calculation.

To obtain the strain energy of each finite element, turn on this option. But this option requires a little more time because the additional calculation is performed.

This option corresponds to [A5] in the 'Advanced options' window.

Default: 0

Initial configuration

○ DO_PART_RELO

Partition and relocation.

To use the partition and relocation approach, turn on this option. Then, a structure will be subdivided and approximately relocated to help the correct configuration in the finite element procedure

Default: 1

Base-pair (BP) and crossover (CO) steps

○ BP_CF_IND

Coefficient function for BP and CO steps (${}^{t}\alpha_{\mathrm{BP}}^{k}$).

This represents the degree of adjusting properties from the initial ($t = 1$) to the final incremental time step ($t = t_f$).

This option corresponds to [B1] in the 'Advanced options' window.

The order of the prebuilt coefficient function is specified. For example, if 1 is specified, the property values are linearly modified. When using the electrostatic interaction option (DO_ES), it is appropriate to specify 2. The coefficient function has a value between 0 and 1 in incremental time steps from 0 to t_f.

[1] Order 1: ${}^{t}\alpha_{\mathrm{BP}}^{1} = 1 - (t - t_f)/(1 - t_f)$

[2] Order 2: ${}^{t}\alpha_{\mathrm{BP}}^{2} = 1 - (t - t_f)^2/(1 - t_f)^2$

[k] Order *k*: ${}^{t}\alpha_{\mathrm{BP}}^{k} = 1 - (t - t_f)^k/(1 - t_f)^k$

Default: 2

○ BP_TIME_FINL

Final incremental time step for BP and CO steps (t_f).

This represents the final incremental time step at which each structural element of BP and CO steps has the final properties. After t_f, the coefficient function has the value 1. t_f should have the value the same or smaller than the total incremental time step (T). If t_f is assigned to 0 or $t_f > T$, t_f is automatically set to T. This option can be used to first converge the mechanical properties and later generate the electrostatic force. For example, setting as $T = 30$, $t_f = 15$, and $t_{\mathrm{ES}} = 10$ represents that the properties of structural elements of BP and CO steps are adjusted for 0-15 incremental time steps, and electrostatic elements are generated for 10-30 incremental time steps.

This option corresponds to [B2] in the 'Advanced options' window.

Default: 0

Single-stranded DNA

○ SS_SAMP

Gaussian sampling of ssDNA properties.

If this option is used, the properties of each ssDNA are sampled.

If not, mean values are used, and their deviation is ignored.

[0] Not sampling

[1] Sampling

This option corresponds to [D1] in the 'Advanced options' window.

Default: 0

○ SS_LCT1_S

Contour length per nucleotide for short ssDNA.
This value represents the length of each nucleotide (nt) for short ssDNA.
Unit = [nm/nt]
This option corresponds to [D2] in the 'Advanced options' window.
Default: 0.38 0.11 (mean, std)

○ SS_LCT1_L

Contour length per nucleotide for long ssDNA.
This value represents the length of each nucleotide (nt) for long ssDNA.
Unit = [nm/nt]
This option corresponds to [D3] in the 'Advanced options' window.
Default: 0.68 0.29 (mean, std)

○ SS_LCT1_k

Coefficient in the model of contour length per nucleotide.
This value represents the modeling coefficient for the contour length per nucleotide.
Unit = [1]
This option corresponds to [D4] in the 'Advanced options' window.
Default: 0.2 0.02 (mean, std)

○ SS_LPB_L

Persistence length for long ssDNA.
This value represents the bending persistence length of long ssDNA.
Unit = [nm]
This option corresponds to [D5] in the 'Advanced options' window.
Default: 0.67 0.15 (mean, std)

○ SS_LPB_ka

Coefficient in the model of persistence length (k_a).
This value represents the modeling coefficient for the contour length per nucleotide.
Unit = [1]
This option corresponds to [D6] in the 'Advanced options' window.
Default: 5.4 0.3 (mean, std)

○ SS_LPB_kb

Coefficient in the model of persistence length (k_b).
This value represents the modeling coefficient for the contour length per nucleotide.
Unit = [1]
This option corresponds to [D7] in the 'Advanced options' window.
Default: 0.21 0.02 (mean, std)

○ SS_EA_L

Stretching rigidity when relaxed.
This value represents the stretching rigidity in the low force region.
Unit = [pN]
This option corresponds to [D8] in the 'Advanced options' window.
Default: 15 2.8 (mean, std)

○ SS_EA_H

Stretching rigidity when stretched.
This value represents the stretching rigidity in the high force region.
Unit = [pN]
This option corresponds to [D9] in the 'Advanced options' window.
Default: 710 60 (mean, std)

○ SS_EA_ka

Coefficient in the model of stretching rigidity (k_a).
This value represents the modeling coefficient for stretching rigidity.
Unit = [1]
This option corresponds to [D10] in the 'Advanced options' window.
Default: 80

○ SS_EA_kb

Coefficient in the model of stretching rigidity (k_b).
This value represents the modeling coefficient for stretching rigidity.
Unit = [1]
This option corresponds to [D10] in the 'Advanced options' window.
Default: 0.072

○ SS_EA_kc

Coefficient in the model of stretching rigidity (k_c).
This value represents the modeling coefficient for stretching rigidity.
Unit = [1]
This option corresponds to [D10] in the 'Advanced options' window.
Default: 1.16

○ SS_GJ_H

Torsional rigidity for short ssDNA.
This value represents the torsional rigidity for short ssDNA.
Unit = [$\mathrm{pNnm^2}$]
This option corresponds to [D11] in the 'Advanced options' window.
Default: 15 3.6 (mean, std)

○ SS_GJ_L

Torsional rigidity for long ssDNA.
This value represents the torsional rigidity for long ssDNA.
Unit = [$\mathrm{pNnm^2}$]
This option corresponds to [D12] in the 'Advanced options' window.
Default: 2 1.2 (mean, std)

○ SS_GJ_k

Coefficient in the model of torsional rigidity.
This value represents the modeling coefficient for torsional rigidity.
Unit = [1]
This option corresponds to [D13] in the 'Advanced options' window.
Default: 0.3 0.12 (mean, std)

○ SS_CF_IND

Coefficient function for ssDNA (${}^{t}\alpha_{ss}^{k}$).

This represents the degree of adjusting properties from the initial ($t = 1$) to the final incremental time step ($t = t_f$).

This option corresponds to [D14] in the 'Advanced options' window.

The order of the prebuilt coefficient function is specified.

[1] Order 1: ${}^{t}\alpha_{ss}^{1} = 1 - (t - t_f)/(1 - t_f)$

[2] Order 2: ${}^{t}\alpha_{ss}^{2} = 1 - (t - t_f)^2/(1 - t_f)^2$

[k] Order k: ${}^{t}\alpha_{ss}^{k} = 1 - (t - t_f)^k/(1 - t_f)^k$

Default: 1

○ SS_TIME_FINL

Final incremental time step for single-stranded DNA (t_f).

This represents the final incremental time step at which each structural element of ssDNA has the final properties. t_f should have the value the same or smaller than the total incremental time step (T). If t_f is assigned to 0 or $t_f > T$, t_f is automatically set to T. After t_f, the coefficient function has the value 1. This option can be used to first converge the intrinsic properties and later generate the electrostatic force. For example, setting as $T = 30$, $t_f = 15$, and $t_{\mathrm{ES}} = 10$ represents that the properties of ssDNA elements are adjusted for 0-15 incremental time steps, and electrostatic elements are generated for 10-30 incremental time steps.

This option corresponds to [D15] in the 'Advanced options' window.

Default: 0

Electrostatic interaction

○ DO_ES

Electrostatic interaction.

If this option is selected, electrostatic elements were generated between two nodes in the cut-off distance.

[0] Not use

[1] Use

Default: 1

○ ES_TEMP

Temperature (T).

This represents the temperature used to determine the Debye screening length.

Unit = [K]

Default: 300

○ ES_MG

Mg condition (C_{Mg}).

This option represents the Mg condition used to calculate electrostatic forces.

Unit = [mM]

This option corresponds to [C1] in the 'Advanced options' window.

Default: 20

○ ES_R_CUT

Cutoff distance (r_{cut}).

The cut-off distance was used as a criterion whether electrostatic elements are generated or not by measuring the distance between nodes in the solution procedure.

Unit = [nm]

This option corresponds to [C2] in the 'Advanced options' window.

Default: 2.5

○ ES_TIME_INIT

Initiating incremental time step of electrostatic interaction (t_{ES}).

For this effective generation of electrostatic elements, t_{ES} can be used as the initiating incremental time step of the electrostatic interaction, which was ignored when the incremental time step was smaller than t_{ES}.

This option corresponds to [C3] in the 'Advanced options' window.

Default: 1

○ ES_CF_IND

Coefficient function for electrostatic elements (${}^t\beta_{\text{ES}}^k$).

This represents the degree of the number of electrostatic elements from the initial ($t = t_{\text{ES}}$) to the final incremental time step ($t = t_f$).

This option corresponds to [C4] in the 'Advanced options' window.

If the structural deformation is expected to be small or large, invoking exponential [1] or linear [3] increase is appropriate, respectively. It is generally sufficient to increase the number of electrostatic elements in a quadratic manner [2].

[1] Exponential: ${}^t\beta_{\text{ES}} = (0.5^{T-t} - 0.5^{T-t_{\text{ES}}})/(1 - 0.5^{T-t_{\text{ES}}})$

[2] Quadratic: ${}^t\beta_{\text{ES}}^2 = (t - t_{\text{ES}})^2/(t_f - t_{\text{ES}})^2$

[3] Linear: ${}^t\beta_{\text{ES}}^1 = (t - t_{\text{ES}})/(t_f - t_{\text{ES}})$

[4] Constant: ${}^t\beta_{\text{ES}}^0 = 1$

Default: 1

○ ES_ITER_NUM

Iteration number for electrostatic interaction.

This represents the iteration number to generate electrostatic elements in each incremental time step. Electrostatic elements were generated uniformly by the number determined by the coefficient function. To avoid the divergence, different configurations were tested by this iteration number for the same number of electrostatic elements.

This option corresponds to [C5] in the 'Advanced options' window.

Default: 3

○ ES_QEFF_USER

User-defined effective charge.
Effective charge (q) value was set to 0.7 and 1.5 for 20 and 100 mM Mg conditions, respectively. In default, the effective charge is determined in terms of Mg condition (C_{Mg}) by a linear function ($q = 0.01C_{\mathrm{Mg}} + 0.5$). This option allows specifying a user-defined effective charge regardless of the Mg condition.
Not to use this option, set 0.
Default: 0

○ ES_CF_USER

User-defined coefficient function for electrostatic elements.
The electrostatic interaction can be controlled by the user-defining coefficient function. Input values should have the same dimension of total incremental time step (T), and each value should be in the range of [0, 1].
For example, for the total incremental time step 10, ES_CF_USER can be set as 0 0.1 0.2 0.4 0.6 0.8 0.9 0.95 0.99 1
Not to use this option, set 0.
Default: 0

Normal mode analysis

○ DO_NMA

Normal mode analysis (NMA).
If this option is selected, NMA is performed after the solution converged.
[0] Not perform NMA
[1] Perform NMA
Default: 0

○ NMA_MODE_NUM

The lowest mode number to be calculated.
Eigenmodes will be calculated from the smallest eigenvalue to this value (excluding rigid-body modes). This mode number should be smaller than the total degrees of freedom (6 × the number of base-pairs).
Default: 200

○ PLOT_NMA_MODE

Plot or save mode shapes.
[0] Not save and not plot
[1] Save and closed (.fig)
[2] Save and opened (.fig)
[3] Save and closed (.png)
[4] Save and opened (.png)
Default: 1

○ PLOT_MODE_NUM

Mode number to be plotted from the lowest mode.
This represents the number of eigenmodes to plot and save from the first mode.
[0] Not save
[k] Save 1 to k modes to fig files
Default: 15

○ XYZ_MODE_NUM

Mode number to save in the XYZ format.
This option indicates the number of eigenmodes from the lowest mode to save as an XYZ file.
[0] Not save
[k] Save 1 to k modes to XYZ files
Default: 15

RMSF and correlation

○ DO_RMSF

Calculation of root-mean-square fluctuation (RMSF) values.
This option indicates whether to calculate the RMSF value for each node. This option works when the NMA option is turned on (DO_NMA = 1).
[0] Not perform
[1] Perform
Default: 0

○ DO_RMSF_CORR

Calculation of correlation coefficients.
This option indicates whether to calculate the Pearson and generalized correlation coefficients for each node. This option works when the NMA option is turned on (DO_NMA = 1).
[0] Not perform
[1] Perform
Default: 0

○ RMSF_CORR_TEMP

Temperature.
This represents the absolute temperature used in the equipartition theorem.
Unit = [K]
Default: 300

○ PLOT_RMSF Plot or save the RMSF distribution.

[0] Not save and not plot

[1] Save and closed (.fig)

[2] Save and opened (.fig)

[3] Save and closed (.png)

[4] Save and opened (.png)

Default: 3

○ PLOT_CORR_P Plot or save the Pearson correlation map.

[0] Not save and not plot

[1] Save and closed (.fig)

[2] Save and opened (.fig)

[3] Save and closed (.png)

[4] Save and opened (.png)

Default: 3

○ PLOT_CORR_G Plot or save the generalized correlation map.

[0] Not save and not plot

[1] Save and closed (.fig)

[2] Save and opened (.fig)

[3] Save and closed (.png)

[4] Save and opened (.png)

Default: 3

Configuration plot

○ PLOT_FINL_CONF Plot or save the configuration at the final incremental time step.

[0] Not save and not plot

[1] Save and closed (.fig)

[2] Save and opened (.fig)

[3] Save and closed (.png)

[4] Save and opened (.png)

Default: 1

○ PLOT_STEP_CONF Plot or save the configurations for all incremental time steps.

The stepwise configurations are saved as fig files.

[0] Not save

[1] Save configuration at each incremental step

Default: 0

Output file

○ GEN_FINL_XYZ
Generation of the xyz file of the final configuration.
[0] Not generation
[1] Generation
Default: 1

○ GEN_STEP_XYZ
Generation of the xyz file for each incremental time step.
[0] Not save
[1] Save configuration at each incremental step
Default: 0

○ GEN_FINL_STL
Generation of the stl file of the final configuration.
[0] Not generation
[1] Generation
Default: 1

○ GEN_STEP_STL
Generation of the stl file for each incremental time step.
[0] Not generation
[1] Generation
Default: 1

○ GEN_FINL_OX
Generation of the oxDNA input file of the final configuration.
The pdb file is generated only when the input CSV file is assigned.
[0] Not generation
[1] Generation
Default: 0

○ GEN_STEP_OX
Generation of the oxDNA input file for each incremental time step.
[0] Not generation
[1] Generation
Default: 1

○ GEN_FINL_PDB
Generation of the pdb file of the final configuration.
The pdb file is generated only when the input CSV file is assigned.
[0] Not generation
[1] Generation
Default: 0

○ GEN_STEP_PDB

Generation of the pdb file for each incremental time step.
[0] Not generation
[1] Generation
Default: 1

○ PDB_OB_IND

Save occupancy and beta as RMSF and strain energy in the pdb file.
This option is used to save the RMSF (occupancy) and residual strain energy (beta) values into the PDB file for visualization. Each value is normalized.
[0] Not save
[1] Save
Default: 1

○ PDB_EX_IND

Export format of the pdb file.
Since the position of central nucleotides of ssDNA does not be determined, they are generated evenly based on the configuration of terminal BPs. The configuration of the generated ssDNA may not be appropriate.
[1] Generation of PDB file except for ssDNA configuration
[2] Generation of PDB file including ssDNA configuration
Default: 1

○ SAVE_MAT_IND

Save of the mat file.
[0] Not save
[1] Save initial and final step data
[2] Save all step data
Default: 1