Exploring Energy Profiles of Random DNA strands

1. Working with pre-defined double helix sequence *ATGCGACT* in a box size 15

A close-up of a bug

Description automatically generated with low confidence

1. Creating the output files trajectory.dat and energy.dat



1. Focusing on the energy.dat

Table

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The columns shown ("Documentation - Oxdna") are:

[time (steps \* dt)] [potential energy] [kinetic energy] [total energy]

Currently, the parameters are:

Graphical user interface, application

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1. Creating plots for time vs each of the 3 columns (seed number 101)

Graphical user interface, chart

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1. Changing seed number from 101 to 105 and observing the output

Graphical user interface, application

Description automatically generated

A lot of noise can be observed so to reduce the noise, we run multiple simulations with different seed numbers and then collate them into a single graph.

1. Chart

   Description automatically generatedChart, line chart

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   Description automatically generatedChart, line chart

   Description automatically generatedChart

   Description automatically generatedFocussing on time vs potential energy, running 5 simulations with different seed numbers.
2. Collating the 5 simulations onto a single graph to get rid of noise.

Chart

Description automatically generated

The above plot was created using manual running of the simulation. Must automate the process so that it runs without having to create 5 different input files and energy files each time. That way 100 simulations (or more) could potentially be run and averaged. Code for the above can be found in Appendix A.

1. An average of 5 simulations with different seed numbers using automated system.

Chart

Description automatically generated

Code for the above can be found in Appendix B.

1. After checking a correct plot was obtained using automated system, an average of 11 simulations was obtained with seed number varying by 2 each time. (Range: 105-85)

Chart

Description automatically generated

1. An average of 16 simulations obtained with seed number varying by 2 each time. (Range: 111-81)

Chart

Description automatically generated

Sources

1. "Documentation - Oxdna". Dna.Physics.Ox.Ac.Uk, 2021, <https://dna.physics.ox.ac.uk/index.php/Documentation#Input_file>.

Appendix A

Graphical user interface, text, application

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Graphical user interface, text, application

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Graphical user interface, text, application

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Graphical user interface, text, application

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Graphical user interface, text, application

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Appendix B

Text

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