# An Educational Tool for Visualize DNA Structures *in vivo*

Shigehiro Fukase $^1$	Masato Wayama $^2$
fukase@mon.hitachi-sk.co.jp	wayama@jomon.ne.jp

- <sup>1</sup> 3rd Application Systems Department, Hitachi Software Engineering Co., Ltd., 5-79, Onoe-cho, Naka-ku, Yokohama 231-0015, Japan
- <sup>2</sup> Open System Sales Department, Bussiness Service Corporation, 2-6-29, Shinmachi, Aomori 030-0801, Japan

## 1 Introduction

Recently, we can use computer graphics and GUI very easily on personal computers. In biology field, many programs are developed to show biochemical molecules. And these are used by many biologists and students.

But, these tools are almost visualize only crystal formed molecules, so it's not help for learning molecules' movement and chemical reactions.

Thus we aim at DNA is balanced with temperature conditions *in vivo*, we developed an simulation tool for DNA's attitude. This tool helps to understanding that molecules are not stable crystal form in nature and molecules' attitude with temperature changes.

## 2 System and Methods

DNA molecules consist of two long chains held together by complementary base pairs [1](Fig. 1). Two chains repeat dissociate and associate while temperature changings because of these are connected with hydrogen bonds between them [3]. A parts which having many A-T pairs dissasociate easily. Because G-C pair is more balanced than A-T pair [2]. This tool diplays DNA's status changes with temperature changings as graphic animations using OpenGL library [4, 5]. And users can set any temperature by thermostatic control bar.

We handle not a static molecule (such as crystal) but dynamic changing model. In this reason, we have to simulate not only structure but also the environment in which molecules exist. If we will have to calculate all actions and desoxyribose's position and movement, calculation and drawing processes are very difficult. So we implemented as easy model with limited information. First, we have to represent to transformation of DNA forms easily. DNAs having phosphatic backbone are represented to geometrical many sided figures. Second, "bracket joint model" is represented to each covalent bonds. Last, And last, hydrogen bonds between base pairs will appears "binding model" with distance between base pairs to calculate DNAs twist easily.

Furthermore, this tool requires less calculation time than calculation time for all vectors of variation. Because, our tool calculates coordinates from probability of changing radius on every temperature.

## 3 Future Works

We developed simplified biochemical simulation system. However, this system will support to learning molecular biologies. Our future objective is to evolve this simulation system. This system will lead to

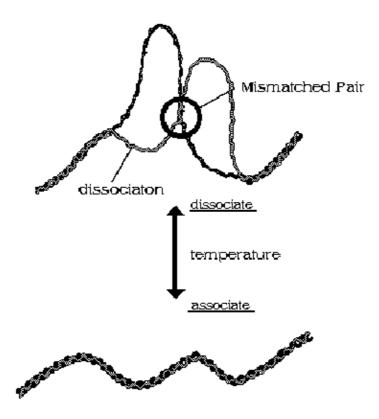


Figure 1: DNA's dissociation and association.

simulate inexpensive molecular biological laboratories, and easy biochemical experiments are going to do in this system.

#### Acknowledgements

The authors would like to thank Shinji Noso of NOSO Institute for his invaluable suggestions, helpful comments and economical supports.

#### References

- Alberts, B., Bray, D. and Lewis, J., Raff, M., Roberts, K., and Watson, J.D., MOLECULAR BIOLOGY OF THE CELL, THIRD EDITION, Garland Publishing, Inc. New York & London, 1983, 1989, 1994.
- [2] Branden, C. and Tooze, J., Introduction to Protein Structure, Garland Publishing, Inc. New York & London, 1991.
- [3] Watson, J.D., Gilman, M., Witkowski, and J., Zoller, M., *Recombinant DNA, second edition*, W. H. Freeman and Company, New York, N.Y. and Oxford.
- [4] Woo, M., Neider, J., and Davis, T., OpenGL Architecture Review Board, three-dimensional structure: The Official Guide to Learning OpenGL, Version 1.1, Addison-Wesley Publishers Japan, January 1997.
- [5] Kilgard, M.J., OpenGL Programming for the X Window System, Addison-Wesley Developers Press, January 1997.