

**THE FLORIDA STATE UNIVERSITY
COLLEGE OF ARTS AND SCIENCES**

COMPUTER VISUALIZATION OF POLYMER CHAINS

By

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INTRODUCTION

Computer visualization is playing a more important role in facilitating exploration, analysis and interpretation of all kinds of data. It offers insight which would be difficult or even impossible to achieve by other means.

A polymer (or macromolecule) is a giant molecule with a very high molecular weight. It consists of many thousands of atoms with the carbon atoms connected by chemical bonds. Polyethylene is one of the most important polymers, which consists of only carbon and hydrogen (C and H) atoms connected through carbon-to-carbon bonds (Figure 1). The molecular formula of the long chain molecule, polyethylene, is C_nH_{2n+2} . In the molten state, polyethylene chains are believed to assume randomly coiled conformations and can be simulated as random walks, see [FY].

Lately the study of polymers has been having a great influence in both natural science and our daily life. The goal of this project is to develop a polymer visualization system that allows convenient specification of polymers and provide tools for the rendering of the specified polymers. These polymers include single polymer chains and those in the liquid-like regions of semicrystalline polymers. It is our hope that by visualizing the graphics of polymers, the conformations of

polymer chains, the entanglements between them, as well as the different mathematical models describing them can be better understood. In this project, we are able to visualize random chain or chains of the polymer polyethylene.

Figure 1 Schematic Representation of a Piece of a Polyethylene Chain

(large dodehedrons — carbon atoms; small dodehedrons — hydrogen atoms.)

CHAPTER 1
POLYMER AND ITS MATHEMATICAL MODELS

Polymer Chain Conformations and Characteristics

As we can see from Figure 1, the polymer (polyethylene) is a long chain molecule which consists of only carbon and hydrogen (C and H) atoms. The carbon atoms are connected through carbon-to-carbon bonds and the adjacent C-C bonds are approximately fixed at the tetrahedral angle (Figure 2). The CH_2 groups of a chain are allowed to rotate around one or more C-C bonds to form numbers of different *conformations*. Conformations are defined as the nonidentical arrangements produced by the rotation of atoms around one or more single bonds.

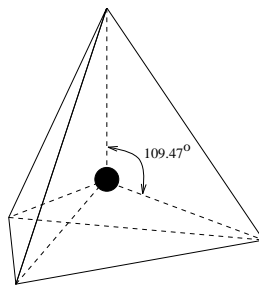


Figure 2 Carbon Atom Centered In a Tetrahedron

The conformations with low energy will be found much more frequently than those

with very high energy. Consider a set of three successive C-C bonds in a chain, the three bonds defines a *rotational state*. The conformational energy of the rotational state has three minima. One occurs with the planar zig-zag conformation (i.e. the rotation angle is zero). The two other minima occur when the third bond is rotated about the mid-bond by 120° and -120° . The corresponding rotational states are designated *trans*, *gauche*⁺, and *gauche*⁻ (Figure 3). It has been found that the probabilities of the rotational states *trans*, *gauche*⁺ and *gauche*⁻ to occur in the *melt* (polymer in the molten state) are given by:

$$p_{trans} = \frac{1 + 2\sigma}{1 + 4\sigma + 2\sigma^2 + 2\sigma^2\omega},$$

$$p_{gauche^+} = p_{gauche^-} = \frac{1 - p_{trans}}{2},$$

where $\sigma = e^{-\frac{E_\sigma}{RT}}$ and $\omega = e^{-\frac{E_\omega}{RT}}$ are functions of the crystallization temperature T in Kelvin scale ($T(K) = T(^{\circ}C) + 273.15$), $R = 1.99$ calories per mole per Kelvin (cal/molK) is the gas constant, E_σ is an energy constant which ranges between 430 calories per mole to 590 calories per mole (cal/mol), E_ω is another energy constant which ranges between 1700 to 2000 cal/mol, see [Flory] or [Duan].

The conformation of a polymer molecule is described by a sequence of the rotational states of carbon bonds. For a polymer chain of $n+2$ bonds, the molecule can assume 3^n distinct conformations. If $n = 10,000$, which represents a modest size chain with molecular weight about 140,000 g/mol, then $3^n \approx 10^{4,771}$! (The Avogadro's number, the number of molecules per mole, is only 6.02×10^{23} /mol.)

i is p_i and the end-to-end distance of this polymer chain is r_i , then we have

$$\langle r^2 \rangle = \sum_i p_i r_i^2.$$

In principle one can obtain $\langle r^2 \rangle$ by counting all the possible conformations, but clearly in practice it is impossible to do. Therefore visualizing the positions of the two end carbon atoms of a chain is among our interests.

Statistics and Entanglements of Polymers in the Liquid-like Region

Semicrystalline polymer formed from the melt generally consists of alternating liquid-like and crystalline regions (Figure 4). In the crystalline regions, polymer chains are packed regularly (Figure 5), while in the liquid-like regions, chains are entangled with each other and assume a random coiled configuration (Figure 6). The crystallites have thicknesses of the order of 100\AA ($\text{\AA} = 10^{-10}\text{meter}$). The other dimensions of the crystallites are much larger. The crystallites invariably take the form of very thin plates or *lamellae*. The thickness of the liquid-like regions is about 30\AA to 180\AA , see [KPM]. So the lengths of the polymer chains (a modest size chain may have length $15,000\text{\AA}$) are many times greater than the lamellar crystal thickness and each molecular chain may traverse the liquid-like regions and pass through one or more lamellae many times, see [FY]. A chain which re-enters the same crystal from which it emerges is referred to as a *loop*. A chain which connects two adjacent crystal lamellae is referred to as a *tie*. A chain

which terminates in the liquid-like region is referred to as a *free-end*.

Experimental results show mechanical properties of semicrystalline polymeric materials depend on topological statistics of polymer chains in the liquid-like regions. For example breaking strength is a function of both the percentages of how many polymers are loops, ties or free-ends in the liquid-like regions and the distributions of chain lengths. As the number of loops increases, so do the number of entanglements among the loops which increases the strength of the material, see [LBH] or [Duan]. Therefore visualizing the polymer chains in the liquid-like region is among our interests.

Figure 4 A Schematical View of Semicrystalline Polymer
(1 — liquid-like region; 2 — interphase; 3 — crystalline region.)

Figure 5 A Schematical View of the Crystalline Region

Figure 6 A Schematical View of the Liquid-like Region

Mathematical Models of Polymer Chains

To obtain a quantitative description of the conformations of polymer chains and the characteristics related to the macroscopic properties, people have developed several different kinds of mathematical models for the polymer chains. Here we introduce the two models used in rendering the polymer chains in the project.

Modified Cubic Lattice Model

Cubic lattice model (see [GDH]) is the simplest lattice model people introduced in studying polymers. In the cubic lattice model polymer chains are simulated as regular random walks on a cubic lattice (Figure 7). Starting from a lattice point,

Figure 7 Cubic Lattice

a walk is continued on the lattice with probability $1/6$ of proceeding to any one of the six possible adjacent lattice points. This model enables people to study polymers quantitatively. However, since it is impossible for two carbon atoms to occupy one site, it would be more satisfactory if polymers are simulated as self-avoiding random walks. *Modified cubic lattice model* is a model developed toward this direction, see [DH]. In the modified cubic lattice model, the cubic lattice idea is retained. The walk is restricted so as to avoid its last step, although it might step on to itself in more than three steps. Starting from a lattice point, a restricted walk is continued on the lattice with a probability $1/5$ of proceeding to any one of the adjacent lattice points except the one it just visited. A single polymer chain of any length in the melt is thus simulated as a restricted random walk on a cubic lattice. In the liquid-like region, polymer chains are simulated as a family of restricted random walks on a cubic lattice between two parallel absorbing boundaries at $z = 0$ and $z = M$. These two boundaries resemble two adjacent crystalline lamellae M units apart. Starting one step away from one of the two boundaries with certain starting probability, a restricted random walk in the family is continued on the lattice until it reaches one of the boundaries or its length limit. A loop is formed if the walk ends at the same boundary as it starts. A tie is formed if a walk ends at the opposite boundary. A free-end is formed if the walk reaches its length limit. The starting probability varies directly with the density of polymers in the liquid-like region. The *length* of a walk is the number

of steps in the walk.

Statistics (Table 1) of polymer chains in the liquid-like region have been calculated therotically assuming the polymer chains long enough so that no free-end occurs, see [DH]. The distribution of loop length and tie length are shown in Figure 8 and 9.

Table 1. Statistics of Random Walks on Cubic Lattice

Statistics	Modified Cubic Lattice Model
Fraction of Loops	$1 - \frac{3}{2M + 1}$
Fraction of Ties	$\frac{3}{2M + 1}$
Average Length of Loops	$2M - \frac{1}{2}$
Average Length of Ties	$\frac{2}{3}M^2 + \frac{2}{3}M - \frac{4}{3}$
Average Length of Walks	$3M - 3$
Variance of Loop Length	$\frac{32M^4 + 112M^3 + 82M^2 + 2M - 15}{15(2M + 1)}$
Variance of Tie Length	$\frac{(M - 1)(M + 1)(56M^3 + 140M^2 + 86M + 45)}{45(2M + 1)}$
Variance of Walk Length	$(M - 1)(2M^2 + 5M + 1)$

Figure 8 Distribution of Loop Length

Figure 9 Distribution of Tie Length

Diamond Lattice Model

The diamond lattice model greatly improves the cubic lattice models by making the geometry more realistic. Cubic lattice model (as well as the modified cubic lattice model) offers an analytic method to calculate the statistics of polymer chains, but it is not entirely satisfactory as a model of real polymers. A polymer molecule is linked through carbon-to-carbon bonds with fixed angles, therefore the most convenient and appropriate lattice to use is the diamond lattice (Figure 10), on which all different conformations of polymer chains fit. A diamond lattice model was introduced for this reason (see [DH]), where polymer chains are simulated as restricted random walks on a diamond lattice.

Figure 10 Diamond Lattice

We now give a brief description of the diamond lattice model. Consider a diamond lattice. The lattice angles of 109.47° resemble the bond angles in polymer chains. The lattice bonds (resembling carbon-to-carbon bonds) of unit length fall into the vector set $\mathbf{B} = \{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4, \mathbf{b}_5, \mathbf{b}_6, \mathbf{b}_7, \mathbf{b}_8\}$, where

$$\begin{aligned}\mathbf{b}_1 &= (0, \sqrt{\frac{1}{3}}, \sqrt{\frac{2}{3}}), & \mathbf{b}_2 &= (0, \sqrt{\frac{1}{3}}, -\sqrt{\frac{2}{3}}), \\ \mathbf{b}_3 &= (0, -\sqrt{\frac{1}{3}}, \sqrt{\frac{2}{3}}), & \mathbf{b}_4 &= (0, -\sqrt{\frac{1}{3}}, -\sqrt{\frac{2}{3}}), \\ \mathbf{b}_5 &= (\sqrt{\frac{2}{3}}, \sqrt{\frac{1}{3}}, 0), & \mathbf{b}_6 &= (\sqrt{\frac{2}{3}}, -\sqrt{\frac{1}{3}}, 0), \\ \mathbf{b}_7 &= (-\sqrt{\frac{2}{3}}, \sqrt{\frac{1}{3}}, 0), & \mathbf{b}_8 &= (-\sqrt{\frac{2}{3}}, -\sqrt{\frac{1}{3}}, 0),\end{aligned}$$

but not all the sequences of the vectors are on the lattice. In particular, a bond vector \mathbf{a} may be followed by another vector \mathbf{b} if and only if $\mathbf{a} \cdot \mathbf{b} = 1/3$. Taking \mathbf{b}_1 and \mathbf{b}_3 as its first two steps, a walk on a diamond lattice is continued with probabilities, p_{trans} or $p_{gauche^{+/-}}$, of proceeding to one of the adjacent lattice points to form a *trans*, *gauche⁺* or *gauche⁻*. Along its way, a sequence of *trans*, *gauche⁺* and *gauche⁻* is formed. In this model, a single polymer chain in the melt is simulated as a restricted random walk on a diamond lattice. It is continued until it reaches the length limit. In the liquid-like regions, polymer chains are simulated as a family of restricted random walks on a diamond lattice between two parallel absorbing boundaries. The two parallel absorbing boundary planes at $z = 0$ and $z = M \cdot \sqrt{\frac{2}{3}}$ resemble the two adjacent crystalline lamellae M bonds apart. Each

of the random walk in the family initiates at a site on one of the boundary plane. The first step of the walk takes either \mathbf{b}_1 or \mathbf{b}_3 with equal probabilities to step into the liquid-like region. We assume that it forms a *trans* with its two preceding bonds inside the crystal (i.e. assume that the interface is normal to the crystalline chains in the crystal). The walk, with each step resembling one carbon-to-carbon bond, is continued on a diamond lattice with probabilities, p_{trans} or $p_{gauche+/-}$, of proceeding to one of the adjacent lattice points until it reaches $z = 0$ (where a loop is formed), $z = M \cdot \sqrt{\frac{2}{3}}$ (where a tie is formed) or its length limit (where a free-end is formed).

The statistics of polymer chains predicated by the diamond lattice model, assuming the polymer chains long enough so that no free-end occurs, are shown in Table **2** through Table **5**, see [Duan].

Table 2. Fractions of Loops and Ties at Different Temperatures

temperature(K)	fractions of loops	fractions of ties
300	$1 - \frac{5.3698}{M} + \frac{21.0335}{M^2} + O(\frac{1}{M^3})$	$\frac{5.3698}{M} - \frac{21.0335}{M^2} + O(\frac{1}{M^3})$
350	$1 - \frac{4.8377}{M} + \frac{16.7557}{M^2} + O(\frac{1}{M^3})$	$\frac{4.8377}{M} - \frac{16.7557}{M^2} + O(\frac{1}{M^3})$
400	$1 - \frac{4.4611}{M} + \frac{14.0158}{M^2} + O(\frac{1}{M^3})$	$\frac{4.4611}{M} - \frac{14.0158}{M^2} + O(\frac{1}{M^3})$
450	$1 - \frac{4.1779}{M} + \frac{12.1127}{M^2} + O(\frac{1}{M^3})$	$\frac{4.1779}{M} - \frac{12.1127}{M^2} + O(\frac{1}{M^3})$
500	$1 - \frac{3.9557}{M} + \frac{10.7141}{M^2} + O(\frac{1}{M^3})$	$\frac{3.9557}{M} - \frac{10.7141}{M^2} + O(\frac{1}{M^3})$
∞	$1 - \frac{2}{M} + \frac{2}{M^2} + O(\frac{1}{M^3})$	$\frac{2}{M} - \frac{2}{M^2} + O(\frac{1}{M^3})$

Table 3. Average Lengths of Loops at Different Temperatures

temperature (K)	expected loop length
300	$1.5346M + 1.6763 - \frac{4.4057}{M} + \frac{4.0565}{M^2} + O(\frac{1}{M^3})$
350	$1.5192M + 1.3774 - \frac{3.6909}{M} + \frac{3.4289}{M^2} + O(\frac{1}{M^3})$
400	$1.5063M + 1.1697 - \frac{3.2052}{M} + \frac{2.9699}{M^2} + O(\frac{1}{M^3})$
450	$1.4953M + 1.0161 - \frac{2.8513}{M} + \frac{2.6247}{M^2} + O(\frac{1}{M^3})$
500	$1.4857M + 0.8975 - \frac{2.5805}{M} + \frac{2.3573}{M^2} + O(\frac{1}{M^3})$
∞	$1.3333M - \frac{0.5}{M} + \frac{0.5}{M^2} + O(\frac{1}{M^3})$

Table 4. Average Lengths of Ties at Different Temperatures

temperature (K)	expected tie length
300	$0.1429M^2 + 1.1194M - 1.3219 - \frac{1.9474}{M} + \frac{7.6278}{M^2} + O(\frac{1}{M^3})$
350	$0.1570M^2 + 1.0877M - 1.2378 - \frac{1.7572}{M} + \frac{6.0861}{M^2} + O(\frac{1}{M^3})$
400	$0.1688M^2 + 1.0608M - 1.1778 - \frac{1.6136}{M} + \frac{5.0697}{M^2} + O(\frac{1}{M^3})$
450	$0.1790M^2 + 1.0377M - 1.1324 - \frac{1.5009}{M} + \frac{4.3513}{M^2} + O(\frac{1}{M^3})$
500	$0.1878M^2 + 1.0173M - 1.0965 - \frac{1.4095}{M} + \frac{3.8176}{M^2} + O(\frac{1}{M^3})$
∞	$0.3333M^2 + 0.6667M - 0.75 - \frac{0.5}{M} + \frac{0.5}{M^2} + O(\frac{1}{M^3})$

Table 5. Average Lengths of Walks at Different Temperatures

temperature (K)	expected walk length
300	$2.3019M - 3.5587 - \frac{11.7728}{M} + \frac{80.3209}{M^2} + O(\frac{1}{M^3})$
350	$2.2788M - 3.3411 - \frac{9.1122}{M} + \frac{56.6040}{M^2} + O(\frac{1}{M^3})$
400	$2.2594M - 3.1838 - \frac{7.4341}{M} + \frac{42.9723}{M^2} + O(\frac{1}{M^3})$
450	$2.2429M - 3.0634 - \frac{6.2844}{M} + \frac{34.2907}{M^2} + O(\frac{1}{M^3})$
500	$2.2285M - 2.9673 - \frac{5.4497}{M} + \frac{28.3533}{M^2} + O(\frac{1}{M^3})$
∞	$2M - 2$

Chapter 2

POLYMER VISUALIZATION SYSTEM

Design of the Polymer Visualization System

Overview

The polymer visualization system is designed to allow convenient specification of polymers and provide tools for rendering the specified polymers. It consists of three main components, the graphic user interface, the polymer generator and the file input and output module as shown in Figure 11. The *graphic user interface* collects commands and specifications of polymers and renders the 3D views of the polymers. The *polymer generator* calculates the coordinates of the polymers. And the *file input and output module* load or save polymers from or to files according to user's instruction.

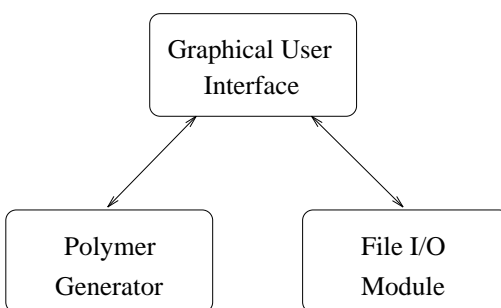


Figure 11 Three Main Components of Polymer Visualization System

Graphic User Interface

Graphic user interface collects commands and specifications of polymers and renders the specified polymers (Figure 12). Its functions include:

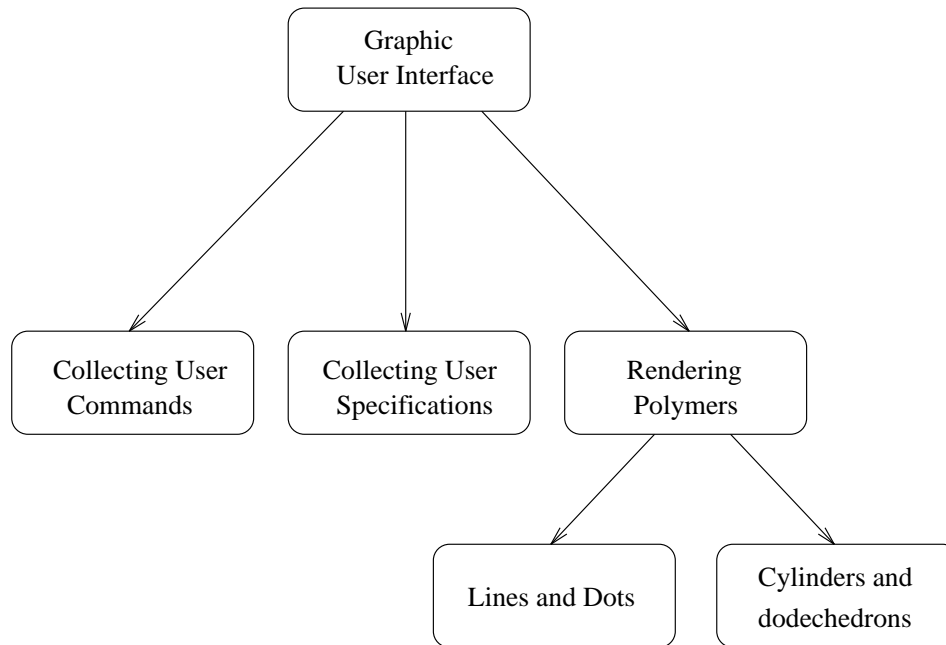


Figure 12 Graphic User Interface

- picking a mathematical model for generating polymers:
the diamond lattice model or the modified cubic lattice model;
- setting polymer parameters:
temperature, length, seed (of random number generator), regionL, regionH, regionW (length, height and width of the liquid-like region) and density;

- rendering polymers:
render polymers as line segments and dots or as cylinders and dodecahedrons.
- adjusting the view of polymers:
shift, rotate, zoom in or out the polymers; clip the polymers outside of the specified liquid-like region; view loops, ties or free-ends separately; reset the view;
- choosing files to save or load;
- providing help:
explain user how to use the system.

Polymer Generator

Following the mathematical models described in the previous section, polymers can be simulated as restricted random walks on either a diamond lattice or a cubic lattice. A random walk starting at one lattice point is continued on the lattice following the rules described. The walk simulating a single polymer chain terminates when it has reached the limited length. For the polymers in the liquid-like region, a family of random walks are generated on the lattice between two absorbing planes. Each walk starts at a lattice point, one unit away from one of the absorbing planes, with certain starting probability and is continued on the lattice until it touches any one of the absorbing planes or its length limit. Figure

13 shows the flow chart of this part.

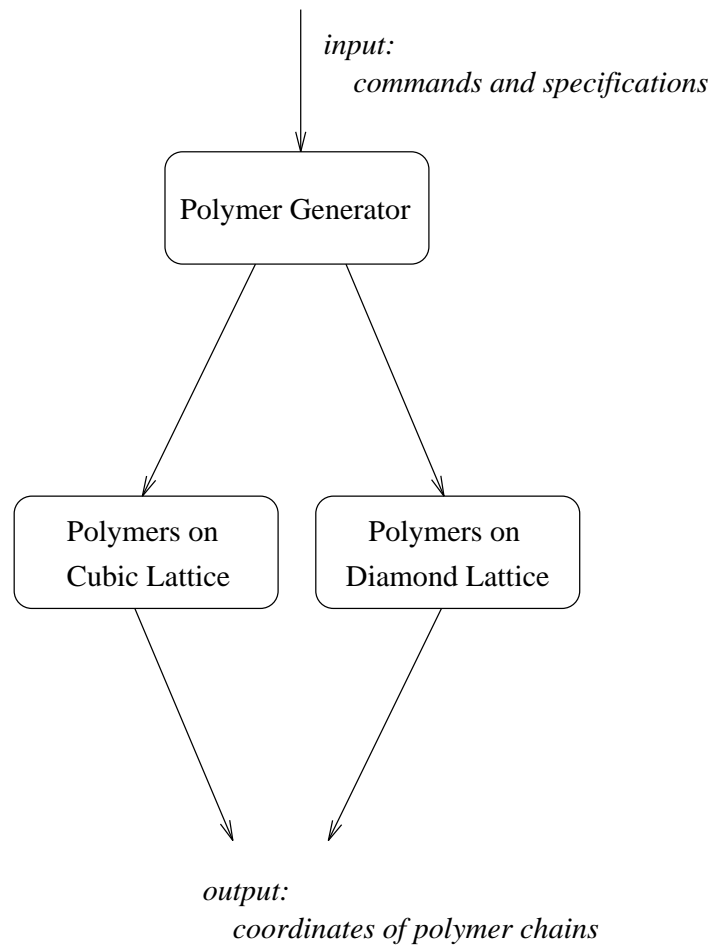


Figure 13 Polymer Generator

File Input and Output Module

This part of the system loads polymer parameters from a text file or saves the polymer parameters and the graphics to files of different formats (Figure 14).

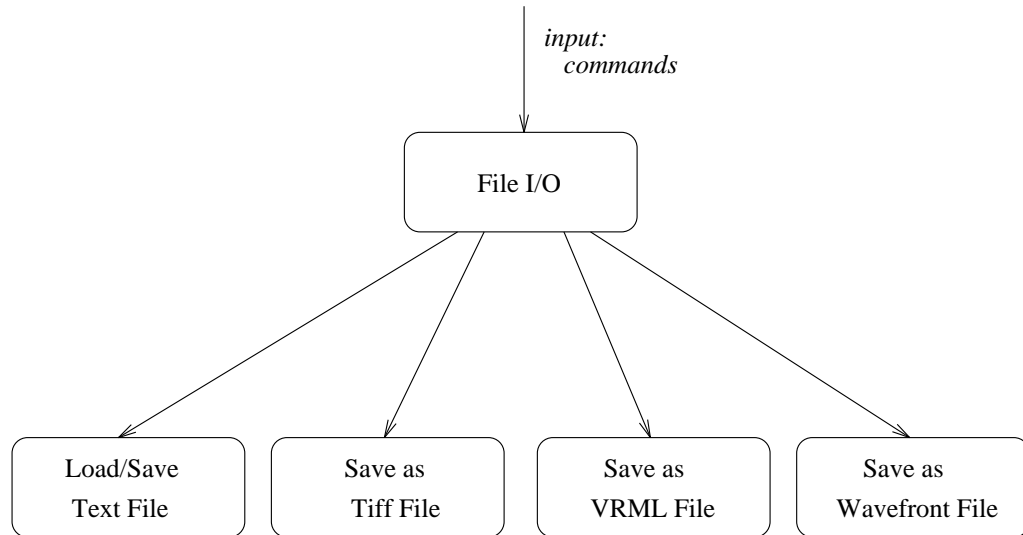


Figure 14 File Input and Output Module

Implementation

Tools and Languages

Tcl and Tk are used in the system for managing the graphic user interphase and Togl and OpenGL for rendering polymers, see [Tcl/Tk] and [OpenGL]. The computations of the system are implemented using C, see [KR].

Tcl (tool command language) is an embeddable scripting language and Tk is a graphical user interface toolkit based on Tcl. Tk defines Tcl commands that allow people to create and manipulate user interface windows. Togl is a Tk widget

for OpenGL rendering, see [Togl]. It allows one to create and manage a special Tk/OpenGL window with Tcl and render into it with a C program.

Graphic User Interface

A top-most main Tk window (*main manager window*) and a togl window (*3D-View window*) are created for managing the graphic user interphase and OpenGL rendering polymers (Figure 15). All the menus are bound on the main manager window to provide Tcl commands. The scales to display the values of polymer parameters and allow user to specify new values. The implementation of main manager window finds its main influence in the similar part of the ShellyLib program of Schultz, see [Schultz]. The Tcl commands are implemented in C. An interpreter is used to point to the data structure manipulated by Tcl and evaluate the Tcl scripts.

Traditionally, carbon atoms and C-C bonds are represented as line segments and dots or circular cylinders and spheres. To get better performance, we used line segments and dots as well as cubic cylinders and dodecahedron to represent carbon atoms and C-C bonds. User may specify to render the cylinders and dodecahedron as wireframes or flat shaded (Figure 16) or smooth shaded objects (Figure 17).

Figure 15 Main Manager Window and 3D-View Window

Figure 16 Cylinders and Dodehedrons with Flat Shading

Figure 17 Cylinders and Dodehedrons with Soomth Shading

Polymer Generator

The Monte Carlo method is used in our system to generate representative chains of polymers with different conformations. The procedure is to draw a sequence of uniformly distributed random numbers between 0 and 1 for each polymer chain. The random numbers so drawn are used to generate a sequence of steps of a random walk, i.e. a sequence of rotational states in diamond lattice model. Each random walk represents one polymer chain. The procedure is implemented using C. A C library function *rand* is used to generate integral random numbers which are then scaled to be uniformly distributed on the interval (0,1).

File Input and Output Module

This part is implemented using C. The format of output file includes: Text, VRML, Tiff (see [Koradi]) and Wavefront. The VRML (Virtual Reality Modeling Language) is a language for describing interactive 3-D objects delivered across the Internet, (see [VRML]). The Tiff is a format for printing. To print a tiff file, one can use the public domain program *xv* or the *netpbm* package by *tiff2pnm* filename | *pnmtops* | *lpr*. And the Wavefront file is the input file format of a Java program which can display 3D wireframes, (see [Wavefront]).

Validation and Verification

Two major goals of any software package are:

To meet its user's needs;

To be error-free.

To make sure the system generates the correct random walks, the approximated statistics of the polymer chains, based on the results of Monte Carlo simulation, were compared and seen to agree with the theoretical statistical results.

A debug button is placed on the main manager window to help further development of the system. It allows the user to input tcl commands and executed.

Chapter 3

RESULTS

The colorful interactive 3-D graphics of polymers rendered by this system are not only pleasing to look at, but also instructive. They can help people to understand features and models of polymer chains and to generate new questions about them. Hence the system is also a part of research, in addition to being an entertaining and educational tool.

The polymer chains that we see using this system are actually mathematical abstractions of polymers — restricted random walks. These random walks are not true self-avoiding random walks which would be a more appropriate mathematical model of polymers. But as we can see from the interactive graphics of these walks, the frequency of self-interaction is small. This observation suggests that simulating polymers as restricted random walks is a reasonable mathematical treatment. While experiencing the polymer visualization system, we also see the loops dominate the liquid-like region as predicated theoretically by both mathematical models. One nice feature of the system is that we can look at the loops, ties and the free-ends separately. We clearly see that the fractions of ties and free-ends in the liquid-like region are quite small when the polymer chains have

a modest length limit (Figure 18). Another intuition we get from the interactive 3D polymer graphics is that the distributions of lengths of loops and ties in the diamond lattice model have the same characteristics as those in the modified cubic lattice model (see Figures 8 and 9). That is the majority of loops are relatively short, although some of the are very long. The lengths of ties have a distribution which is not unlike the one in Figure 9. We hope our intuition can be later confirmed theoretically.

Figure 19 show the temperature effects on the chain conformations. We see, at a higher temperature, that a polymer chain is more likely to be coiled together and the end-to-end distance is shorter than at a lower temperature where it is more likely to be stretched out and the end-to-end distance is longer.

Another use of the system is as a teaching aid. For example, it draws the three basic conformations of polymers and both cubic and diamond lattices. Figure 20 shows the three rotational states of three carbon-to-carbon bonds.

Chapter 4

USER MANUAL

The Polymer Visualization System

The Polymer Visualization System is a piece of computer software which allows for convenient specification of polymers and renders 3D views of polymers, which can be both single polymer chains or those in the liquid-like regions of semicrystalline polymers. It uses OpenGL or Mesa, Togl, Tcl and Tk and C. It was built and tested on Unix.

Getting Started with Polymer Visualization System

Graphic User Interface

The Polymer Visualization System is a graphical based program with menus, buttons, sliders and it has a 3D window which interacts with user via the mouse and keyboard. It opens with two visible main windows: the Main manager Window and the 3D-View Window. [Windows for help and debugging can be activated when needed.] All the controls and polymer graphs appear within these two windows on the screen. Both of the windows are resizable. The Keyboard is used to enter numbers and commands. Functions are mouse activated although some can be activated from keyboard as well.

- **Main Manager Window**

This window is used to issue controls as shown in Figure 21. It consists of a menu bar, which includes eight pull down menus (File, Export, Polymer, Model, Render, View, Teaching-aids and Help) and a debug button, list of polymer parameters, number boxes, minimum values of polymer parameters, scales, maximum values of polymer parameters, calibrators and a scroll bar.

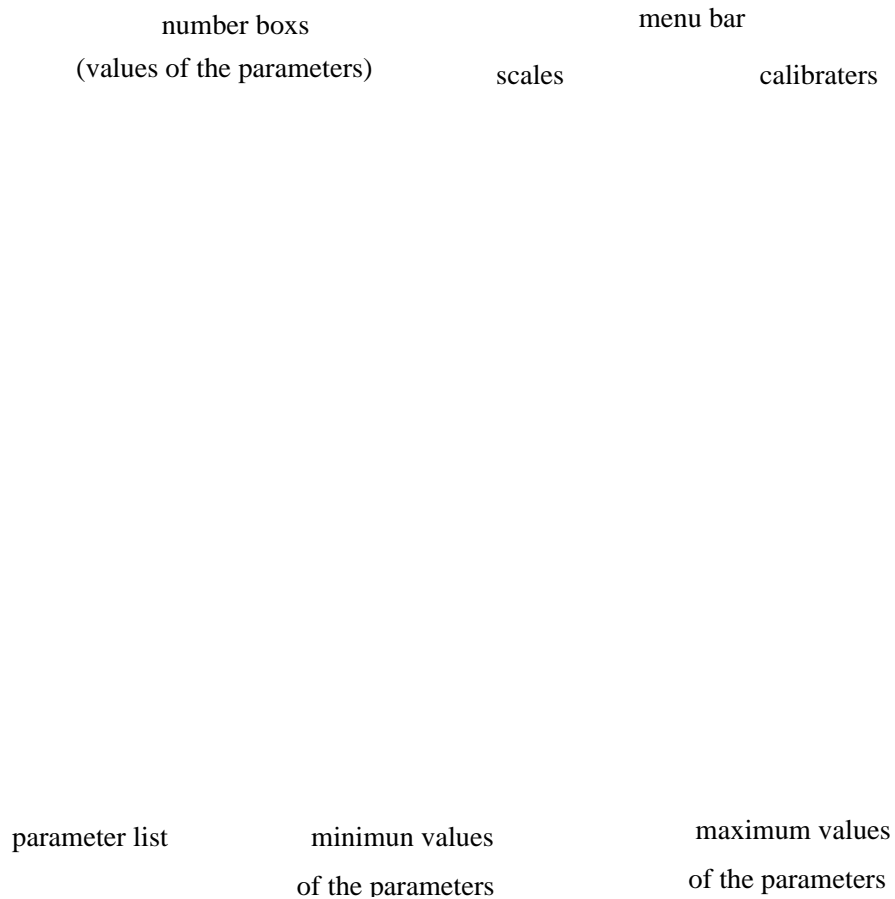


Figure 21 Main Manager Window

- **3D-View Window**

This window is used to display the specified polymers as shown in Figure 22.

Figure 22 3D-View Window

- **Keyboard**

Keyboard is used to enter numbers and commands. The following are keyboard shortcuts available with the Polymer Visualization System.

◇ when the mouse pointer is in the main manager window:

Ctrl-l — load polymer parameters from a file;

Ctrl-s — save polymer parameters in a file;

Ctrl-r — reset the view;

Ctrl-q — quit from the system;

F1 — open Tutorial window;

F10 — evoke File menu;

Alt+first letter of a menu — evoke the menu;

◇ when the mouse pointer is in a scale:

→ or ↓ — increase the value of the variable;

← or ↑ — decrease the value of the variable;

◇ when the mouse pointer is in a pull down menu:

↓ — point to a menu item below;

↑ — point to a menu item above;

→ — switch to a pull down menu at right;

← — switch to a pull down menu at left;

◇ when the mouse pointer is in the 3D-View window:

+ or ↑ — zoom in;

- or ↓ — zoom out;

↑ — move the graph +1 unit in z-direction;

↓ — move the graph -1 unit in z-direction;

- — rotate polymer graph about z-axis clockwise;
- ← — rotate polymer graph about z-axis anticlockwise.

- **Mouse**

Polymer Visualization System uses a three button mouse to press controls. Its function are shown in Figure 23.

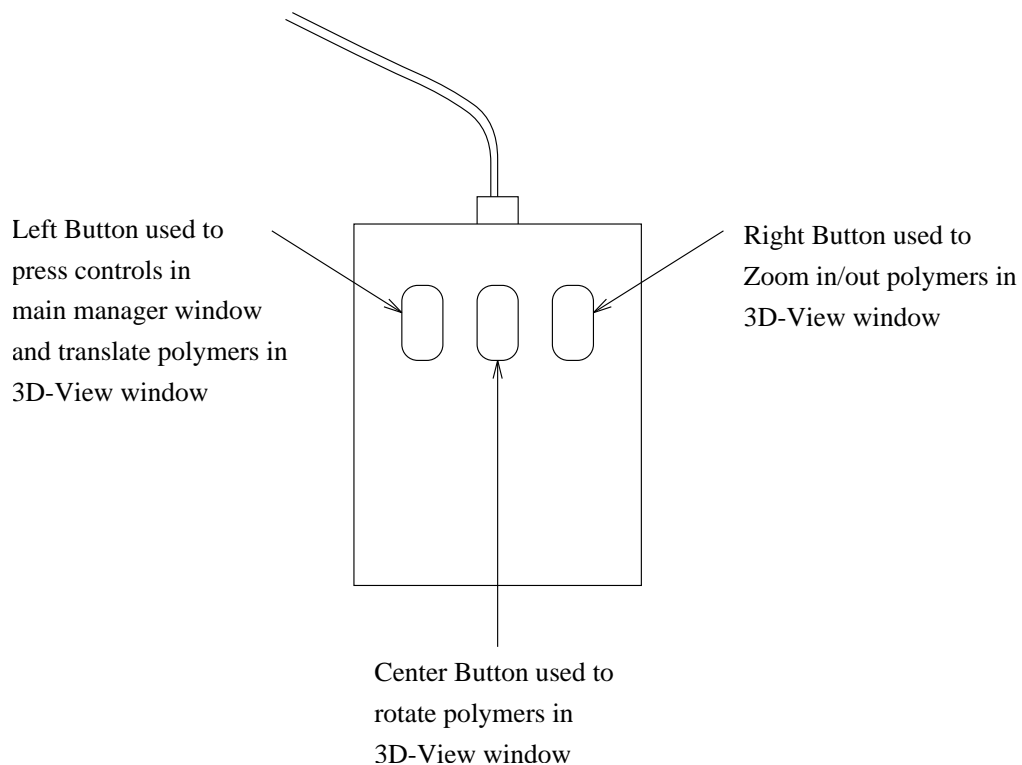


Figure 23 The Mouse and its Functions

Using Menu

To use a menu, press the right mouse button on a menu name. A pull down menu will pop up. Drag the mouse pointer to the desired menu item and release the button. Alternatively, one can use the keyboard shortcut Alt + the underlined letter of the menu name to select menu and ↓ or ↑ to select the desired menu item.

The items of eight pull down menus are shown in Figure **24**.

Figure 24 Main Manager Window and the Eight Menus

Using Controls

- Scroll Bar — displays an arrow at each end and a rectangular slider which moves in a track. It is always associated with a control area such as entry or listbox which may be larger than space allowed in a displaying window. One can adjust the view by clicking mouse button 1 on the arrows or by dragging the slider;
- Scale — It has a slider moving in a track, much like a scroll bar. It is used to select a value of a variable from a range. The position of the slider indicates the value. To move the slider to a new value, pick up the slider and drag it to the desired value.
- Number box — contains the value of a parameter and also indicates the position of the slider in the scale next to it. To edit the value, click the box and type number on the keyboard to replace the old one or by dragging the slider in the scale next to the number box.
- Calibrater — It is denoted by a "Cal." button. It is used to control the maximum and the minimum values of a variable whose value is shown in a number box and a scale. To modify the values, click on the button and change values in a seperate window poped up.
- Radio Button — It has a diamond shape and appears on a pull down menu. It provide a way to select one of a group mutually exclusive values of one

attribute. Each radio button in a group is associated with one of the value (see Figure 24).

- Check button — It has a square shape and appears on a pull down menu also. It is used to control some attributes which have only two values 0 and 1 (see Figure 24).
- Debug Button — is used to set values of parameters through keyboard and assist one to modify the system;

Saving Parameters or Images to Files

By selecting or entering the file name, one can save the polymer parameters or images as text files, VRML files, Tiff files or Wavefront files. To save the parameters to a text file, one can select the file by first clicking on *File* menu and choose *save*. A file window will pop up, one can enter the file name (*unnamed.ch2* by default) or click on the file name if it is in the window or use scroll bar to get the file name displayed on the window and then click on it. After selecting the file name, proceed by clicking Ok button. To save polymer image to a VRML, Tiff or Wavefront file, one need click on *Export* menu. And then proceed as just described.

Loading Parameter Files

By selecting the file name, one can load the polymer parameters from a file. To

select the file, first clicking on *File* menu and choose *load*. A file window will pop up, one can choose the file as described in the last paragraph. The desired polymer parameters and the graph will be shown up in the main manager window and the 3D-View window.

On-line Help

There is an on-line help built into the system to help user get started using Polymer Visualization System. One may leave the help window on while experiencing the polymer lab.

Figure 25 Tutorial Window

Understand Menu Items and Polymer Parameters

Menu Items

The Polymer Visualization System has eight menus. Each of them has several items. The following is the list of the menu items and their functions.

- File
 - ◊ Load — load polymer parameters from a text file;
 - ◊ Save — save polymer parameters to a text file;
 - ◊ Quit — quit from the system;
- Export
 - ◊ VRML — save polymer graph image as a VRML file;
 - ◊ Tiff — save polymer graph image as a Tiff file;
 - ◊ Wavefront — save polymer graph image as a Wavefront file;
- Polymer
 - ◊ Single Chain — generate a single polymer chain;
 - ◊ Liquid-like Region — generate polymers in a liquid-like region;
- Model
 - ◊ Cubic — choose modified cubic lattice model;
 - ◊ Diamond — choose diamond lattice model;
- Render

- ◇ Line — render polymers as line segments and dots;
- ◇ Wireframe — render polymers as wireframes of cubic cylinders and dodehedrons (effective for single chains only);
- ◇ FlatShaded — render polymers as flat shaded cubic cylinders and dodehedrons (effective for single chains only);
- ◇ SmoothShaded — render polymers as smooth shaded cubic cylinders and dodehedrons (effective for single chains only);
- View
 - ◇ Show hydrogens too — show hydrogen atoms also in the 3D-View window (effective for diamond lattice model and single chains only);
 - ◇ Show All — show all polymer chains (loops, ties and free-ends) in the 3D-View window (effective for liquid-like region only);
 - ◇ Loop Only — show only loops in the 3D-View window (effective for liquid-like region only);
 - ◇ Tie Only — show only ties in the 3D-View window (effective for liquid-like region only);
 - ◇ Free-end Only — show only free-ends in the 3D-View window (effective for liquid-like region only);
 - ◇ AutoUpdate — allow update the view automatically;
 - ◇ DrawCoordSys — draw coordinate system;
 - ◇ SetClip — clip out chains at the outside of specified volume (effective for

- liquid-like region only);
- ◇ DoubleSide — generate polymer chains from both planes (effective for liquid-like region only);
- ◇ ColorRevert — revert the background color of the 3D-View window;
- ◇ ResetView — reset the view in the 3D-View window;
- ◇ ClearScreen — clear the graphs in the 3D-View window;
- teaching-aids
 - ◇ polymers — view polymer(s) (default);
 - ◇ cubic lattice — view cubic lattice;
 - ◇ diamond Lattice — view diamond lattice;
 - ◇ trans — view a piece of polymer chain in trans conformation;
 - ◇ gauche⁺ — view a piece of polymer chain in gauche⁺ conformation;
 - ◇ gauche⁻ — view a piece of polymer chain in gauche⁻ conformation;
- help
 - ◇ Tutorial — a simple tutorial manual;
 - ◇ About Polymer laboratory — copy right of the system;

Polymer Parameters

- length — maximum length of a polymer chain;
- temperature — crystallization temperature (effective for diamond lattice

model only);

- seed — a seed for a new sequence of random numbers;
- regionL — the thickness of the liquid-like region (effective for liquid-like region only);
- regionH — the height of the liquid-like region (effective for liquid-like region only);
- regionW — the width of the liquid-like region (effective for liquid-like region only);
- density(%) — density of polymers in the liquid-like region (effective for liquid-like region only);

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APPENDICES

A. Makefile and Header File

A.1. Makefile

A.2. polymerl.h

B. Source Code of Common Functions

B.1. polymerl.c

C. Source Code of Graphic User Interface

C.1. Lab.tcl

C.2. Lab.c

C.3. render.c

C.4. hydrogen.c

C.4. teaching_aid.c

D. Source Code of Polymer Generator

D.1. gen.c

E. Source Code of File Input and Output

E.1. rdwrt.c

E.2. screenDump.c