Solving SATISFIABILITY with Molecular Algorithms

by

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Abstract

Molecular computation uses techniques from molecular biology and combinatorial chemistry to perform generalized computations. We explore, via simulation, three distinct molecular algorithms for solving SATISFIABILITY. The simulation measures the number of molecular operations for solving SATISFIABILITY. The test input consists of a set of random 3-SAT instances distributed over a range of clause-variable ratios ($\alpha = [0.2, 14.0]$).

Contents

Chapter 1

Introduction

Molecular computing uses parallel interactions between genetic molecules, such as DNA or RNA, to perform computational tasks. We provide an experimental system for simulating three molecular algorithms. In this chapter we discuss the process of solving a combinatorial problem with both standard or molecular models of computation. This discussion includes an introduction to simulating molecular algorithms. We conclude the chapter with the contents of this report.

1.1 Introduction to molecular computation

NP-complete problems, such as SATISFIABILITY, may be verified in polynomial time with the aid of a short proof called a *witness*; NP-complete problems may be solved by checking the state for all possible *witness candidates*. In a standard computing environment, brute force search can check all 2^n witness candidates in exponential time.

Molecular computing requires exponential space to represent all witness candidates. This combinatorial space of witness candidates can be filtered in polynomial time with parallel molecular operators.

Conjunctive normal form (CNF) can be used to represent SATISFIABILITY instances as a structured input format for Boolean formulas. A CNF expression ϕ consists of a conjunctive set of m Boolean disjunctive clauses. The expression ϕ consists of n independent Boolean variables. We have, e.g.,

$$\phi = C_1 \wedge C_2 \wedge \cdots \wedge C_m,$$

where each clause C_i contains k disjunctive Boolean variables

$$C_i = (v_1 \vee v_2 \vee \cdots \vee v_k).$$

A potentially satisfying witness for a SATISFIABILITY instance is a Boolean assignment to the variables that make the formula true. Such a witness can be represented as an n-bit

Boolean vector. Validating a witness candidate for a SATISFIABILITY instance may be verified in polynomial time with CHECKSAT(ϕ, B) (Algorithm 1.1.1 below). CHECKSAT(ϕ, B) iterates over each of the clauses C in the expression ϕ. The *test_clause* variable gets set to $False$, assuming that the clause cannot be satisfied. If the clause can be satisfied with the input configuration B, then the algorithm continues. If each of the m clauses can be satisfied, then CHECKSAT(ϕ, B) returns $True$; otherwise the algorithm returns $False$.

Algorithm 1.1.1: CHECKSAT(ϕ, B)

```
for each clause $C$ in $\phi$
  do { $test\_clause \leftarrow False$
       for each variable $v$ in $C$
         do { if $v \in B$
                then $test\_clause \leftarrow True$
       if $test\_clause = False$
         then return ($False$)
return ($True$)
```

Algorithm 1.1.2: BRUTESAT(ϕ)

```
$n$ number of variables in $\phi$
$t$ is bit vector representing a witness candidate

for $t \leftarrow 0$ to $2^n - 1$
  do { if CHECKSAT($\phi, t$)
         then return (SATISFIABLE)
return (UNSATISFIABLE)
```

CHECKSAT(ϕ, B) may be applied as a subroutine in a brute force SATISFIABILITY solver. Algorithm 1.1.2 provides pseudocode for a brute force SATISFIABILITY solver BRUTESAT(ϕ). The algorithm BRUTESAT(ϕ) tests a maximum of 2^n Boolean configurations, using the CHECKSAT(ϕ, B) algorithm. If the test configuration t satisfies the input instance ϕ, then the algorithm returns `SATISFIABLE`; otherwise the algorithm returns `UNSATISFIABLE`.

In this project, we consider molecular algorithms to solve SATISFIABILITY. Molecular algorithms permit many combinations to occur in parallel [1, 15]. This permits molecular operations, such as *append* or *extract*, to perform in parallel on all of the string contents of a test tube [1, 15, 12]. In Chapter 3, we explore techniques from combinatorial chemistry to generate combinatorial sets [15, 9, 12]. The function COMBINATORIALGENERATE(n), which we introduce in Chapter 3, constructs an exponential number of configurations in linear time.

Let us consider Algorithm 1.1.3 as a simplified version of Lipton's algorithm [15, 12].

Algorithm 1.1.3: ExtractSat(ϕ)

```
$n$ number of variables in $\phi$

$T \leftarrow$ CombinatorialGenerate($n$)
for each clause $C$ in $\phi$
    do
        $T_C \leftarrow \emptyset$
        for each variable $v$ in $C$
            do
                $T_T \leftarrow \text{extract}(T, v)$
                $T_C \leftarrow \text{mix}(T_C, T_T)$
        $T \leftarrow T_C$
if $T = \emptyset$
    then return (UNSATISFIABLE)
return (SATISFIABLE)
```

ExtractSat(ϕ) collects configurations satisfying Boolean variables from each clause in ϕ. Initially, ExtractSat(ϕ) constructs a combinatorial space T with the subroutine CombinatorialGenerate(n). The initial space T contains configurations representing all potential witness candidates for ϕ. The space T gets filtered for each clause to only those configurations that satisfy any of the Boolean variables contained within a clause. These potential solutions are incrementally mixed into the tube T_C for each clause. Once extracting the contents for the current clause C the tube T_C of partial assignments gets stored as T. The set T now contains all witnesses that can be satisfied with the previous clauses. If T contains no string configurations after filtering variables for each clause, then ϕ is `UNSATISFIABLE`; otherwise ϕ is `SATISFIABLE`, and T contains configurations for all satisfying witnesses.

We consider Lipton's algorithm in detail in Chapter 3. However, the ExtractSat(ϕ) function provides an introductory view of a molecular algorithm. ExtractSat(ϕ) differs from BruteSat(ϕ) in the method of determining the state for a Satisfiability instance. With the BruteSat(ϕ) algorithm, exponential configurations get generated in exponential time; on the other hand, with ExtractSat(ϕ) exponential configurations get filtered from exponential space.

1.2 Simulation of molecular Satisfiability solvers

We consider three molecular algorithms for solving Satisfiability: Lipton's algorithm [15], Ogihara and Ray's algorithm [18, 19], and a new algorithm, introduced here, that we call the 'Distribution' algorithm. Lipton's algorithm begins with a combinatorial space of all n-bit witness candidates and filters the combinatorial space so that only those that satisfy the input formula remain. Ogihara and Ray's algorithm constructs a space of witness candidates with a heuristic search. The Distribution algorithm expands a set of witnesses with non-conflicting variables from each clause. Chapters 3 and 4 discuss the implementation of these algorithms.

This project introduces a system for simulating three molecular algorithms for solving Satisfiability. The system provides standard operations for molecular computing that we introduce in Chapter 2. It also records runtime metrics, including counts of molecular operators, solution memory footprints, and execution times. These metrics let us analyze algorithmic performance of each molecular algorithm.

Molecular Simulation, the simulation system introduced in this project, automates execution of DIMACS CNF instances. Simulation of each of the algorithms measures metrics for a set of randomly generated 3-Sat expressions. The 3-Sat instances span discrete clause-variable ratios from 0.2 to 14.0 in increments of 0.2, creating a sweep of Satisfiability instances. This experimental setup generates Satisfiability problem instances with both `SATISFIABLE` and `UNSATISFIABLE` configurations.

1.3 Report Overview

In the following chapters, we describe molecular algorithms for solving Satisfiability. We begin, in Chapter 2 with an introduction to gene sequencing technologies and molecular biology. The background continues with definitions of molecular operations for operating on DNA or RNA. Next, we introduce Satisfiability with as a language and as a Boolean circuit. We describe equivalent encodings and classifying characteristics for Satisfiability.

Chapters 3 and 4 introduce each of the three molecular algorithms for solving Satisfiability. In Chapter 3, we discuss Lipton's [15, 12] and Ogihara and Ray's [18, 19, 25] algorithms for Satisfiability. The chapter concludes with existing simulations and physical implementations of these molecular algorithms. Chapter 4 introduces the Distribution algorithm.

Chapters 5 and 6 discuss the project implementation. In Chapter 5, we introduce Molecular Simulation and describe algorithm invocation. Chapter 6 describes the experimental workflow for importing Satisfiability instances for each of the three molecular algorithms under test.

Chapter 7 provides a discussion of algorithm metric performance based on execution test results. Chapter 8 concludes with the contributions of this project and future directions for molecular computation.

Chapter 2

Background

This chapter provides a background on molecular computation techniques. We begin with an introduction to nanotechnology and then provide an example of encoding information with molecular matter. Following this example, we introduce Adleman's molecular operators for solving an instance of HAMILTONIAN PATH. The operators provide a base instruction set for molecular computing, and provide the primitives to construct molecular algorithms.

In the second half of this chapter, we provide an introduction to SATISFIABILITY. We define SATISFIABILITY as a circuit. We then view SATISFIABILITY as a language. We also discuss practical matters related to efficiently evaluating SATISFIABILITY, such as how to encode input and output, and how to classify instances of SATISFIABILITY for the test cases that we consider.

2.1 On nanotechnology and construction of molecules

Richard Feynman founded the field of nanotechnology in his 1959 talk 'There's Plenty of Room at the Bottom' [6]. Examples of applied nanotechnology include the manufacturing of graphene [23] and DNA nanopores [16]. Graphene consists of a planer arrangement of carbon atoms that provides desirable physical and electrical properties [23]. DNA nanopores create a physical channel reading genetic sequences [10]. Gene sequencing technologies provide an example of applied nanotechnology [10, 14, 20].

Smaller and cost-effective DNA sequencers provide the ability to read the contents of a gene. Benchtop sequencers [14, 20] allows doctors to treat patients at the genome level from their office. Life Technologies and Oxford Nanopore offer gene sequencers based on solid-state semiconductor technology [14, 20].

2.2 On microbiology and computation

Microbiology studies the interactions among organic molecules. In this project, we explore techniques from applied genetics as a means for generalized computation. Molecular computation encodes data as sequences of DNA or RNA.

Strings of nucleotides encode information as oligonucleotides. A *oligonucleotide* is a short string of genetic information. There are several configurations for DNA and RNA; these include +RNA, −RNA, +DNA, −DNA, ±RNA, ±DNA, and +mRNA [2]. The polarity of the DNA sequence denotes the direction of genetic information. +DNA gets denoted by $5'$—$3'$ and −DNA gets denoted by $3'$—$5'$. We focus on +DNA and −DNA as a substrate for encoding configurations for computational states.

Arbitrary encodings that represent mappings from variables to physical oligonucleotides may have undesirable structure and functionality. Conventional techniques for DNA computing employ variable mappings from a library of oligonucleotides.

Let us consider two techniques for representing information with oligonucleotides. These allow us to encode integer mappings as a fixed width integer sequence.

Representing an integer sequence requires a systematic mapping of an oligonucleotide entry with an integer counterpart. A fixed width representation map independent sequences on a readable boundary. Now we explore an example for encoding an integer sequence with a sequence of oligonucleotides. A sample mapping is provided in Table 2.1.

Table 2.1: A mapping of the integers $[0, 5]$ with arbitrary oligonucleotide definitions.

Integer	**Oligonucleotide**	**Reverse-complement**
0	$5'$`TCTCCC`$3'$	$3'$`AGAGGG`$5'$
1	$5'$`AAACCC`$3'$	$3'$`TTTGGG`$5'$
2	$5'$`GGTAAA`$3'$	$3'$`CCATTT`$5'$
3	$5'$`CCCTCC`$3'$	$3'$`GGGAGG`$5'$
4	$5'$`CTTTTC`$3'$	$3'$`GAAAAG`$5'$
5	$5'$`CCTTCC`$3'$	$3'$`GGAAGG`$5'$

Suppose that we would like to encode the sequence of integers S as an equivalent oligonucleotide representation O_1.

We have, e.g.,

$$S = [1, 3, 4, 3, 2, 0]$$

and

$$O_1 = 5'\texttt{AAACCC} \mid \texttt{CCCTCC} \mid \texttt{CTTTTC} \mid \texttt{CCCTCC} \mid \texttt{GGTAAA} \mid \texttt{TCTCCC}3'.$$

Recovering the sequence S from O_1 can be done several ways. Because the definition of the sequence exists, we may use the reverse complement to match sequences. Another method splits the sequence O_1 on the encoding width. In this case, the encoding width is six base pairs. Gene sequencing tools permit reading the sequence and interpretation of the data with Table 2.1.

Molecular computing encodes genetic information for both storage and operations on a problem state. These interactions include matching and replication. Although this setting describes and artificial construction for a machine, the natural encodings of organisms also share the mechanics that we exploit. Interactions of molecules provide mechanics for generalized computation with oligonucleotides.

In the following chapters, we describe molecular algorithms for SATISFIABILITY and provide insight to construction of a generalized molecular computer. Next we provide a toolbox for molecular computation. The tools presented permit generalized computation with molecular biology techniques. In the next section we introduce the techniques from Adleman's molecular toolbox [1].

2.3 Adleman's molecular toolbox for solving HAMITONIAN PATH

Leonard Adleman performed the first molecular computation in 1994 with recombinant DNA in a bench laboratory setting [1]. This experiment solved a six vertex instance of HAMILTONIAN PATH, an NP-complete problem. In this section, we describe the techniques used in this experiment. We provide definitions for the following operations from Adleman's molecular toolbox: append, extract, mix, split, and purify.

Definition HAMILTONIAN PATH
Given an undirected graph G, does there exist a path that visits every vertex exactly once?

Adleman's encoding for graphs uses oligonucleotides for defining each vertex. The vertex representation shares a similar definition for our example of encoding a sequence of integers in Table 2.1. Representing edges requires a definition of a reverse-complement oligonucleotide; this string connects the suffix of the vertex v_i with the prefix of v_j. For example, let us consider an example for appending v_2 to v_1. Let, e.g.,

$$v_1 = 5'\texttt{ATCTTT}3'$$
$$v_2 = 5'\texttt{CCTATA}3'.$$

From the definition of v_1 and v_2, we can construct an edge $e_{1,2}$ as

$$e_{1,2} = 3'\texttt{AAAGGA}5'.$$

Appending v_2 to v_1 gets accomplished by first attaching the edge $e_{1,2}$ to the vertex v_1

```
5'ATCTTT3'
   3'AAAGGA5'.
```

Next we attach v_2 to the resulting complex, yielding

$$\begin{array}{l} 5'\texttt{ATCTTT|CCTATA}3' \\ \quad\;\; 3'\texttt{AAAGGA}5'. \end{array}$$

Finally the edge may be removed and we have the sequence

$$v_1 \cdot v_2 = 5'\texttt{ATCTTT|CCTATA}3'.$$

The sequence $v_1 \cdot v_2$ represents the path v_1 to v_2, and can be obtained with the *append* operation. A test tube T stores possible solutions. The tube T starts as an empty tube. For solving HAMITONIAN PATH, we introduce equimolar portions of each oligonucleotide vertex for a starting configuration with the *mix* operation.

Definition *Mix*
$T \leftarrow \text{mix}(T_1, \ldots, T_n)$ — combine n test tubes of information. The output consists of a single set $T = T_1 \cup \cdots \cup T_n$.

A small initial set may be amplified with *polymerase chain reaction* (PCR). PCR thermocycles the contents of the tube to replicate the contents. Introducing the each vertex representation to the contents randomly generates all potential paths. We create this representation elongating the initial vertex with a fixed path length.

Append attaches a string to each string contained in a test tube. *Split* portions a tube into multiple portions. We will use split-mix synthesis as a technique for generation of combinatorial space in Chapter 3.

Definition *Append*
$T' \leftarrow \text{append}(T, s)$ — the concatenation of the oligonucleotide s with each element in T.

Definition *Split*
$[T', T''] \leftarrow \text{split}(T)$ — distributes T into two tubes. Each of the resulting tubes, T' and T'', contain the same representative elements of T.

The initial and terminal conditions for the graph get fulfilled by extracting, from the tube T, only paths that begin with V_{in} and end with V_{out}. Extracting only strings from T that match these conditions constrain the number of potential strings to only those that satisfy the conditions of the graph instance.

Definition *Extract*
$T' \leftarrow \text{extract}(T, s)$ — separates all oligonucleotides from T containing the sequence s. The output consists of a set T' of those oligonucleotides containing s.

The tube T consists of possible encodings that have the correct starting and ending vertices. We select only strings with length n, where n is the number of vertices in G, to ensure that all vertices get traversed. This can be performed with *gel electrophoresis*, a technique for sorting molecules by mass. Next, we ensure that each vertex occurs exactly once. This gets accomplished by extracting possible vertices. If a vertex occurs multiple times in a path, then the string representation gets discarded.

Finally, we check T with *detect* to determine if any valid paths remain. If valid paths exist, then each string may be read for the path assignment.

Definition *Detect*
detect(T) — determine if any encodings are present in T. The output consists of $true$ or $false$, for $T \neq \emptyset$ or $T = \emptyset$ respectively.

2.3.1 Additional molecular operators

In the following chapters, we will use the molecular operators for construction of molecular Satisfiability solvers. The Distribution algorithm, introduced in Chapter 4, requires the *splice* operation.

Definition *Splice*
$[a_1, a_2] \leftarrow \text{splice}(a, b)$ — cuts an oligonucleotide a with a subsequence b into two pieces by a restriction enzyme. These two pieces are a_1 and a_2.

In the implementation of a simulation system, we avoid redundant string representations with the *purify* operation. This is a synthetic version of PCR. Purify balances the space representation of molecules with a uniform distribution.

Definition *Purify*
$T' \leftarrow \text{purify}(T)$ — provides a uniform distribution from the contents of T as T'.

2.4 Definition of Satisfiability

Satisfiability is a canonical NP-complete language. Each Satisfiability instance efficiently encodes a set of conditions to satisfy. Because Satisfiability is NP-complete, it can be reduced to any NP-complete language.

Definition Satisfiability
Formally defined as the language

$$\text{Satisfiability} = \{\langle \phi \rangle \mid \phi \text{ is a satisfiable Boolean formula}\}[22].$$

Evaluation of a SATISFIABILITY instance requires validating the input with the instance definition. We introduce SATISFIABILITY evaluation with a circuit. Let us consider a three-layered circuit for SATISFIABILITY. This circuit consists of n inverters, m **OR** gates, and one **AND** gate with m-fan-in. This circuit behaves according to the internal wiring of the input expression ϕ. Figure 2.1 contains a schematic for SATISFIABILITY.

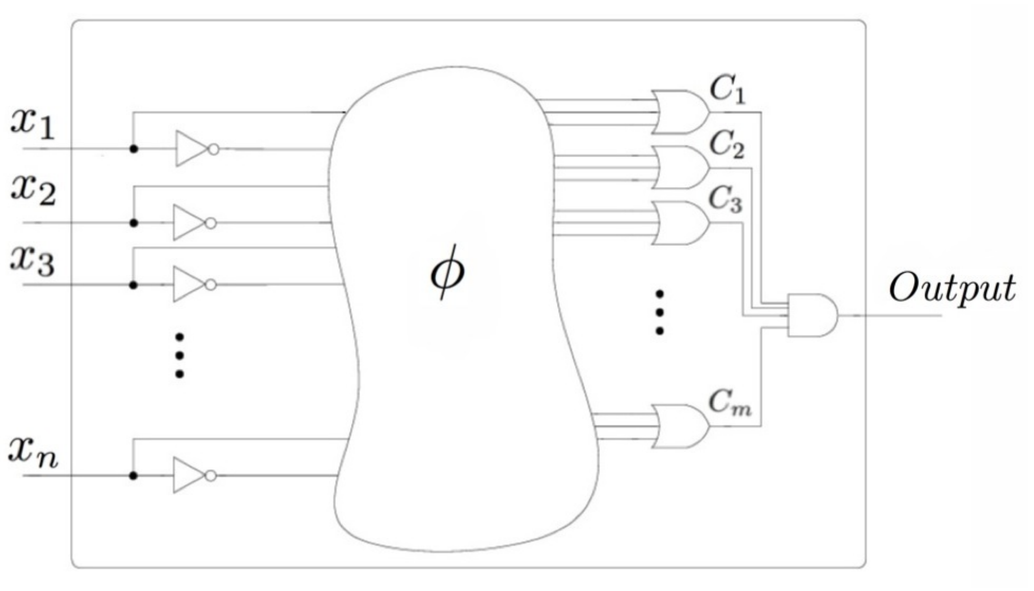

Figure 2.1: A circuit describing SATISFIABILITY.

The realization of SATISFIABILITY as a circuit shows two insights of the problem. SATISFIABILITY can be implemented with logic components proportional to the problem size, and the worst case verification consists of enumerating all possible switch configurations. SATISFIABILITY as a language demonstrates that it is equivalent to all other NP-complete languages.

Cook and Levin independently introduced the canonical instance of a NP-complete language SATISFIABILITY[3, 13]. A NP-complete language is one that is in NP and NP-hard. A NP-hard language is at least as hard as any problem in NP.

The next section considers standards adopted for SATISFIABILITY. This allows practitioners to apply SATISFIABILITY in various settings.

2.5 Evaluating SATISFIABILITY

In this section, we describe two standards for encoding the SATISFIABILITY problem that we adopt for the implementation. This includes the input and output standards for the

Satisfiability Competition [4, 21].

Next, we introduce problem instance classification for Satisfiability. Classification of Satisfiability problem instances include randomly generated, combinatorial, and industrial [21]. The experimental setup in Chapter 6 considers generation of random k-Sat input.

2.5.1 Input and output

Each year a competition showcases techniques for evaluating Satisfiability [21]. We conform to the standards of the Sat Competition `http://www.satcompetition.org/`. Sat solvers demonstrate state-of-the-art techniques for solving three main tracks of Satisfiability instances. The tracks exhibit applications for Satisfiability, including: industrial applications, hard combinatorial, and random problem instances.

The input and output standards for Satisfiability allow common benchmarks for Sat solvers.

Input

DIMACS CNF provides a standard input for Satisfiability [4]. The format permits sharing of existing Satisfiability benchmarks by encoding Satisfiability in conjunctive normal form (CNF). The format is user readable with a natural encoding for Satisfiability. We provide an example of this encoding in Section 5.6.

Output

Sat Competition output consists of the status for a DIMACS CNF input instance [21]. This includes the known state, either `SATISFIABLE`, `UNSATISFIABLE`, or `UNKNOWN`. When a witnessing satisfying assignment occurs, the assignment gets provided as a list of integers with the `SATISFIABLE` state. We provide an example along with a custom interface in Section 5.7.

2.5.2 Metrics for classifying Satisfiability

Sat phase transition and Sat backbones are two classifying metrics for Satisfiability. These metrics may be used to classify Satisfiability expressions. We will use these metrics in the next section for defining a collection of random k-Sat instances.

Definition CNF
Conjunctive Normal Form consists of the intersection of sets of disjunctive literals.

Definition k-CNF
Consists of a CNF expression with each disjunctive clause containing k literals.

Definition k-SAT
Problem variant of SATISFIABILITY where each clause consists of k Boolean literals. k-CNF formula provide an equivalent representation.

Definition SAT phase transition
The SAT phase transition is a region where both satisfiable and unsatisfiable instances are likely. The ratio of clauses to variables $\alpha = m/n$ provides a characterization for where phase transitions may occur in the space of all k-CNF formula [5, 11].

Definition SAT backbones
SAT backbones are the variable assignments present in all of the satisfying assignments to a SATISFIABILITY expression [26]. This is a set of variables that occur in all satisfiable witnesses for an input expression.

2.5.3 SATISFIABILITY instances

There are several methods for constructing SATISFIABILITY instances. We consider techniques for constructing instances based on random assignment, combinatorial, and real applications from industry. The instance type demonstrate properties of SATISFIABILITY and provide heuristics for certain input.

A random k-SAT expression consists of m clauses with k literals per-clause from n variables [24]. Variable assignments get distributed with probability

$$Prob\left(\frac{1}{n}\right).$$

The positive or negative variable polarity get assigned with a probability

$$Prob\left(\frac{1}{2}\right).$$

Combinatorial instances provide difficult benchmark cases. These instances can be converted from other NP-complete problems. This category also includes games and graph theoretic problems represented as SATISFIABILITY.

Industrial processes apply SATISFIABILITY in many real world problems. This includes circuit layout, planning, logistics, circuit fault testing and many other industrial NP-complete problems. Applications for industrial SAT will often apply heuristics, and approximation techniques to relax the problem. This allows approximate solutions to be computed in an efficient amount of time.

Chapter 3

Existing molecular algorithms for Satisfiability

In this chapter, we introduce two molecular algorithms for Satisfiability. These algorithms are distinct in the resolution of a Satisfiability instance. Lipton's algorithm requires a space to be constructed before execution, where Ogihara and Ray's algorithm constructs a valid space during execution. Following the description, we explore the physical implementation and simulation of these algorithms.

3.1 Lipton's algorithm for Satisfiability

Introduced in 1995 by Richard Lipton [15], this algorithm creates an exponential search space for the CNF expression. Each variable gets evaluated with the combinatorial space, reducing the space on each iteration. The satisfiable configurations are present in the remaining space. This algorithm is analogous to a conventional brute-force search for all solutions.

3.1.1 Description of Lipton's algorithm

Lipton's algorithm consists of two main procedures. The first phase constructs a combinatorial space of 2^n independent vectors. Second, the combinatorial space gets filtered based on the input CNF instance.

The function Combinatorial Generate(n) implements the split-mix synthesis technique [8, 9]. It returns a gel consisting of 2^n independent oligos that correspond to a unique vector space. The space begins construction with an initial medium. An iterative loop elongates a growing solution with the split-mix synthesis. Each split corresponds with appending the tubes with a truth and false assignment. The two tubes are mixed and amplified to contain equimolar portions.

The amplification process gets modeled with a purification step. This eliminates all redundant strings for the simulated implementation. After the iteration completes, the complete combinatorial space gets returned. This space consists of 2^n vectors of length n.

From the combinatorial space, we will begin to filter satisfying solutions to the input CNF formula. For each clause, we extract each of the variables present in the solution space. A disjunctive set T_C contains the satisfied string instances for each clause. Lipton's Algorithm iterates over each of the clauses. From the selected clause, the variables get extracted from the combinatorial space. Once complete, the remaining space, T, contains satisfiable instances for ϕ.

3.1.2 Pseudocode for Lipton's algorithm

Algorithms 3.1.1 and 3.1.2 provide pseudocode for Lipton's algorithm. Appendix B lists a detailed execution trace for Lipton's algorithm.

Algorithm 3.1.1: Combinatorial Generate(n)

```
$T_{comb} \leftarrow \emptyset$
$T_{comb} \leftarrow \text{mix}(T_{comb}, start)$
for $v \leftarrow 1$ to $n$
    do $[T_1, T_2] \leftarrow \text{split}(T_{comb})$
       $T_1 \leftarrow \text{append}(T_1, +v)$
       $T_2 \leftarrow \text{append}(T_2, -v)$
       $T_{comb} \leftarrow \text{mix}(T_1, T_2)$
return $(T_{comb})$
```

Algorithm 3.1.2: Lipton's Algorithm(ϕ)

```
$n$ number of variables in $\phi$
$T \leftarrow$ Combinatorial Generate($n$)
for each clause $C$ in $\phi$
    do $T_c \leftarrow \emptyset$
       for each variable $v$ in $C$
           do if $v$ is a positive literal
                then $T_P \leftarrow \text{extract}(T, +v)$
                     $T_c \leftarrow \text{mix}(T_P, T_c)$
                else $T_N \leftarrow \text{extract}(T, -v)$
                     $T_c \leftarrow \text{mix}(T_N, T_c)$
       $T \leftarrow T_c$
return $(\text{detect}(T))$
```

3.2 Ogihara and Ray's algorithm for Satisfiability

Ogihara and Ray's algorithm consist of a breadth-first evaluation of clauses from a CNF formula [18, 19]. The algorithm constructs a set of potential solutions based on parsing a 3-CNF formula. In this section, we describe the preconditions and execution of Ogihara and Ray's algorithm.

3.2.1 Description of Ogihara and Ray's algorithm

Prior to execution of the algorithm it requires two attributes of CNF input:

1. All clauses consist of exactly three literals
2. All clauses must be sorted by variable

Attribute (1) gets fulfilled by considering only 3-Sat expressions. If models of k-Sat with $k > 3$, then a polynomial time reduction to 3-Sat must occur prior to execution.

Attribute (2) gets fulfilled by sorting the clauses prior to execution; providing the weak ordering

$$v_1 < \cdots < v_n,$$

where the polarity of each variable may consist of a positive or negative assignment.

The initial tube consists of potential states for the first two variables.

Expanding each partial assignment iterates over each clause in the input CNF. Construction of satisfiable expressions consider the possibilities of the clause ordering

$$x_u < x_v < x_w.$$

Ogihara and Ray's Algorithm evaluates each subsequent variable and determines possible assignments. The possible assignments for the variables v_1 and v_2 get extracted if v_3 matches. Effectively pruning only potential solutions. These potential solutions T_P and T_N get appended with the positive or negative string assignments. The algorithm continues until each variable gets evaluated. The remaining space T contains all solutions for the CNF instance ϕ after the algorithm terminates.

3.2.2 Pseudocode for Ogihara and Ray's algorithm

Algorithm 3.2.1 provides pseudocode for Ogihara and Ray's algorithm. Appendix B lists a detailed execution trace for Ogihara and Ray's algorithm.

Algorithm 3.2.1: OGIHARA AND RAY'S ALGORITHM(ϕ)

```
$n$ number of variables in $\phi$
Each variable of the reordered clause can be accessed by $v_1$, $v_2$, and $v_3$

Reorder variables by most frequent to least frequent literal appearance
Reorder each clause in increasing literal order

$T \leftarrow \{[+x_1 \cdot +x_2], [+x_1 \cdot -x_2], [-x_1 \cdot +x_2], [-x_1 \cdot -x_2]\}$
for each variable $x_i$ in $3 \leq i \leq n$
  do
    $[T_P, T_N] \leftarrow \text{split}(T)$
    for each clause $C$ in $\phi$
      do
        $[v_1, v_2, v_3] \leftarrow C$
        if $x_i = v_3$
          then
            $T_{P1} \leftarrow \text{extract}(T_N, v_1)$
            $T_{N1} \leftarrow \text{extract}(T_N, -v_1)$
            $T_{P2} \leftarrow \text{extract}(T_{N1}, v_2)$
            $T_N \leftarrow \text{mix}(T_{P1}, T_{P2})$
        if $\neg x_i = v_3$
          then
            $T_{P1} \leftarrow \text{extract}(T_P, v_1)$
            $T_{N1} \leftarrow \text{extract}(T_P, -v_1)$
            $T_{P2} \leftarrow \text{extract}(T_{N1}, v_2)$
            $T_P \leftarrow \text{mix}(T_{P1}, T_{P2})$
    $T_P \leftarrow \text{append}(T_P, +x_i)$
    $T_N \leftarrow \text{append}(T_N, -x_i)$
    $T \leftarrow \text{mix}(T_P, T_N)$
return (detect($T$))
```

3.3 Implementations of molecular SATISFIABILITY solvers

In this section, we describe physical and simulated implementations for molecular SATISFIABILITY algorithms. This includes simulation of Lipton's and Ogihara and Ray's algorithms. We see a physical implementation of Ogihara and Ray's algorithm with manual laboratory procedures.

3.3.1 Physical implementations

Yoshida and Suyama implemented Ogihara and Ray's algorithm with manual molecular biology techniques [25]. This experiment solved a 3-CNF instance with four variables and 10 clauses.

3.3.2 Simulations

Martn-Mateos et al. introduced a simulation for Lipton's algorithm [17]. Molecular operations get implemented with ACL2, a Common Lisp variant. The framework for this system implemented test cases for Lipton's algorithm.

Ogihara provides test results for implementation of his original molecular algorithm [18]. This simulation provides a comparison with Lipton's algorithm for practical length restrictions.

Chapter 4

A new molecular algorithm for Satisfiability

This chapter introduces a new molecular algorithm for Satisfiability. The distribution algorithm parses an input CNF expression into growing and self regulated set of possible combinations.

4.1 Distribution algorithm for Satisfiability

The distribution algorithm parses an input CNF expression into growing and self regulated set of possible combinations. A possible combination begins with all members of the first clause. Variables get inserted into an expanding set of valid assignments. A clause gets eliminated when an assignment contains a conflict.

4.1.1 Description of the Distribution algorithm

Initially the algorithm starts with the variable assignments of a clause. Evaluation of subsequent clauses extends the solution space with the Insert Variable subroutine. During each insertion, the variable gets inserted into a potential solution vector. Table 4.1 lists the four possibilities for variable assignment.

Table 4.1: Configurations for the Insert Variable subroutine

Case	Return state	State
1	$v \cdot s$	if v is less than all elements in s
2	$s \cdot v$	if v is greater than all elements in s
3	$s_1 \cdot v \cdot s_2$	if v is between two elements in s
4	$\emptyset$	if v conflicts with $-v$ in s
5	s	if v exists in s

During this phase, each variable from a disjunctive clause gets considered, incrementally constructing a partial solution space. Cases (1), (2), and (3) place a variable v into an existing sequence s. Each of these cases represents when the variable v get inserted in a non-decreasing sequence.

A variable conflict occurs when both positive and negative assignments of a variable occur in a sequence s. In this case (4), the sequence s gets removed from the set potential solutions. If the sequence s contains the variable v, case (5), then the existing sequence s gets returned unmodified.

Redundant vectors get removed after insertion of the next disjunctive clause. Any remaining witnesses in the solution space contain non-conflicting variable assignments. This does not immediately require that each witness to be a complete satisfiable assignment. Satisfiable witnesses remain in a non-empty satisfying solution space.

Vectors that are of equal magnitude of the number of variables in the problem instance are satisfiable witnesses. However, there may exist solutions that span only the required satisfiable assignments; that is activate each of the independent clauses with at least one non-conflicting assignment. This assignment may be the minimum witness for the expression, in the case that the backbone consists of the variables of the maximum witness.

4.1.2 Pseudocode for Distribution algorithm

Algorithms 4.1.1 and 4.1.2 provide pseudocode for the Distribution algorithm. Appendix B lists a detailed execution trace for the Distribution algorithm.

Algorithm 4.1.1: INSERT VARIABLE(T, v)

```
$T_R \leftarrow \emptyset$
**for each** string $s$ in $T$
  **do** {
    **case** (1) : $v < s$
      **then** $s' \leftarrow \text{append}(v, s)$
    **case** (2) : $v > s$
      **then** $s' \leftarrow \text{append}(s, v)$
    **case** (3) : $s_1 < v < s_2$
      **then** {
        $[s_1, s_2] \leftarrow \text{splice}(s, v)$
        $s_1 \leftarrow \text{append}(s_1, v)$
        $s' \leftarrow \text{append}(s_1, s_2)$
      }
    **case** (4) : $\neg v \in s$
      **then** $s' \leftarrow \emptyset$
    **case** (5) : $v \in s$
      **then** $s' \leftarrow s$
    $T_R \leftarrow \text{mix}(T_R, s')$
  }
**return** $(T_R)$
```

Algorithm 4.1.2: DISTRIBUTION SAT(ϕ)

```
$m$ number of clauses
$k$ number of variables in each clause

Initialize with the variables from the first clause
$T \leftarrow \{C_1\}$
**for** $i \leftarrow 2$ to $m$
  **do** {
    $T_C \leftarrow \emptyset$
    **for each** variable $v$ in $C_i$
      **do** {
        $T_I \leftarrow$ INSERT VARIABLE$(T, v)$
        $T_C \leftarrow \text{mix}(T_C, T_I)$
      }
    $T \leftarrow T_C$
  }
**return** $(detect(T))$
```

Chapter 5

Molecular Simulation: A system for molecular computation

This chapter introduces Molecular Simulation: A system for molecular computation. We provide an overview of the software and download location for Molecular Simulation and its documentation. We provide tools for use with Molecular Simulation. This includes Perl execution scripts and visualization for output data. We provide examples for Molecular Simulation's input and output. Invocation of Molecular Simulation from the command line provides user configurable options. The next chapter describes the usage of Molecular Simulation with automated execution.

5.1 Overview

Molecular Simulation provides a molecular lab for operating on DNA. The present simulation implements three molecular algorithms for SATISFIABILITY. The included `Perl` scripts process DIMACS CNF input directories with invocations to Molecular Simulation.

Molecular Simulation may be executed directly or invoked with the assistance of an execution script. The system requirements to execute or design a molecular experiment are listed in this section.

This program is a simulated molecular lab for experimenting with DNA operations. Implementation of three molecular algorithms for solving SATISFIABILITY include Lipton's algorithm, Ogihara and Ray's algorithm, and the Distribution algorithm. Chapters 3 and 4 provide a background and pseudocode for these algorithms.

5.2 Download

Molecular Simulation can be downloaded from:
`https://github.com/dncarley/MolecularSimulation`.

5.3 Requirements

Requirements for Molecular Simulation are specified in this section. This includes the hardware and software requirements for running Molecular Simulation on your system.

5.3.1 Hardware requirements

Molecular Simulation requires a 64-bit processor with 2 GB of RAM.

5.3.2 Software requirements

`gcc` (GNU Compiler Collection) must be installed on your system.

`Perl` must be installed on your system to automate build and execution of Molecular Simulation.

5.4 Documentation

The project website contains detailed documentation for Molecular Simulation. The documentation provides an overview of Molecular Simulation that may be used independently of Chapters 5 and 6 for getting started. The online documentation provides detailed datatype, function, and class definitions.

5.5 Tools

This project uses several tools for automating tasks and execution. In this section, we introduce tools to automate execution and visualize output from Molecular Simulation.

5.5.1 Perl utilities

The source directory includes several `Perl` scripts to assist in building and initiation of tests for Molecular Simulation. Table 5.1 documents the basic usage for build and testbench execution scripts. Each script provides detailed execution options.

5.5.2 Data Visualization

A Sat datapoint visualization for Molecular Simulation's output can be downloaded from:
`https://github.com/dncarley/VisualizeSatDatapoints`
Ben Fry's example in Chapter 4 of *Visualizing Data* [7] provides a framework for importing output from Molecular Simulation. The visualization project directory contains a README for usage.

Table 5.1: `Perl` execution commands and descriptions.

Perl script	**Usage**	**Description**
`build.pl`	`$ perl build.pl`	Compiles Molecular Simulation and generates an executable in the directory `./execute/simulation`.
`buildGenerate.pl`	`$ perl buildGenerate.pl`	Generates a sweep of CNF formulas over a range of k-SAT ratios. Program uses a modified random k-SAT generator from Microsoft Research.
`executeMolecularSat.pl`	`$ perl executeMolecularSat.pl`	Executes Molecular Simulation for a directory of SATISFIABILITY expressions with desired algorithms. If no options are specified, then each of the three algorithms are executed and output is generated in the same test directory.
`runSimulation.pl`	`$ perl runSimulation.pl`	Executes `build.pl` followed by `executeMolecularSat.pl`. Any command line arguments get passed to `executeMolecularSat.pl`

5.6 Input

Input to Molecular Simulation consists of a DIMACS CNF file. The definition of the `*.cnf` filetype can be accessed from: `ftp://dimacs.rutgers.edu/pub/challenge/satisfiability/doc/`.

```
c comments begin with a ‘c’
c
c cnf input is designated with ‘p cnf’
c    followed by number of variables <n>, and clauses <m>
c
p cnf <n> <m>
c
c A clause is represented by a sequence of <k> integers,
c     separated by whitespace and ending with a ‘0’.
c Each variable is represented by the integer sequence,
c    negative polarity is represented by ‘-’.
c
-3 9 14 0
6 -9 -12 0
-2 11 17 0
3 -13 -17 0
```

5.7 Output

Output from Molecular Simulation, by default, conforms to the 2011 SAT Competition rules. The rules can be accessed from: `http://www.satcompetition.org/2011/rules.pdf`.

```
c comments begin with a ‘c’
c
s SATISFIABLE
c
c A line beginning with a ‘s’ marks the status.
c This can be either ‘UNSATISFIABLE’, ‘SATISFIABLE’, or ‘UNKNOWN’.
c
v -3 -9 11 13 0
c
c A satisfiable witness begins with a ‘v’ and ends with a ‘0’.
c     A sequence of integers, between ‘v’ and ‘0’, encodes a satisfiable assignment.
```

Table 5.2 describes an extended custom output. This output reports parameters for metric performance evaluation.

Table 5.2: Molecular Simulation output logging.

Parameter	**Description**
`c algorithmType:`	Display the algorithm type: `Lipton`, `Ogihara-Ray`, `Distribution`
`c algorithmTime:`	Display the algorithm execution time in seconds.
`c solutionMemory:`	Display the solution space memory footprint in Bytes.
`c mixCount:`	Display the number of `mixes` required during algorithm execution.
`c extractCount:`	Display the number of `extracts` required during algorithm execution.
`c appendCount:`	Display the number of `appends` required during algorithm execution.
`c splitCount:`	Display the number of `splits` required during algorithm execution.
`c spliceCount:`	Display the number of `splices` required during algorithm execution.
`c purifyCount:`	Display the number of `purifications` required during algorithm execution.
`c numVar:`	Display the number of `variables` in the input CNF expression.
`c numClause:`	Display the number of `clauses` in the input CNF expression.

5.8 Execution

Invocation of Molecular Simulation can be performed from the command line.

```
$ ./execute/simulation i [input] [options]
```

The `[input]` consists of a DIMACS CNF file. Command line `[options]` may be a combination of the options in Table 5.3.

Table 5.3: Command line options for Molecular Simulation

Argument	**Parameters**	**Description**
`-a`		Algorithm select
	`d`	Distribution algorithm
	`l`	Lipton's algorithm
	`o`	Ogihara and Ray's algorithm
`-d`		Debug
`i`		Input
	`[input]`	DIMACS CNF file
`-w`		Write output to file
	`[output]`	Output filename

Let us consider an example. Suppose that we would like to execute Ogihara and Ray's algorithm for a DIMACS CNF file. We would like to execute the instance `test1.cnf` located in the directory `/molecularSimulation/testbench`. We output the results `test1-o.out` in the same directory as the input CNF. We invoke Molecular Simulation with the following command.

```
$ ./execute/simulation i ../testbench/test1.cnf -a o -w ../testbench/test1-o.out
```

In the next chapter, we will describe the automation for a random k-SAT sweep with each of the algorithms. The provided Perl scripts are the recommended method for building and execution of Molecular Simulation.

Chapter 6

Experimental Setup

This chapter describes the use of Molecular Simulation for evaluation of a set of DIMACS CNF SATISFIABILITY instances. We discuss configuration for generation of random k-SAT instances. Further, any existing DIMACS CNF benchmark may be imported for test. We provide example configuration options for automating the execution of Molecular Simulation. The example continues with an analysis of runtime metrics for each test instance. The next chapter provides the results from the k-SAT sweep experiment.

6.1 Setup

In this section, we describe prerequisites for executing a test bench with Molecular Simulation. Molecular Simulation requires a 64-bit architecture with a UNIX like system with `gcc` and `Perl`. The target system must meet the minimum requirements.

Building Molecular Simulation can be performed by invoking the `Perl` script `build.pl` from the command line.

```
$ perl build.pl
```

This script generates an executable `simulation` in the directory `molecularSimulation\execute`. The next sections describe invocation of Molecular Simulation with desired options. We begin with the creation and importation of DIMACS CNF datasets.

6.2 Create dataset

We will create a sweep of random k-SAT instances to observe SAT phase transition. David Wilson's `ksat.c` generates random k-SAT instances in DIMACS CNF format. The program takes four arguments to create a unique DIMACS CNF instance. Invocation of the program can be performed with the following command.

```
./execute/ksat k n m s > output.cnf
```

This generates *output*`.cnf` in DIMACS CNF format with k variables per clause n variables, m clauses, and random seed s.

We use automated `Perl` scripts to create a sweep of DIMACS CNF instances. Setup for a sweep configuration includes specifying a set of ratios. Invocation of the script generates a set of random k-SAT instances. The redirected output gets stored in the target directory with the previous file naming convention. We use the following command to invoke the construction of a sweep of k-SAT instances.

```
$ perl buildGenerate.pl
```

6.3 Import dataset

Datasets of DIMACS CNF input may be provided for batch processing. This includes random k-SAT instances generated from the previous section, or importing existing DIMACS CNF instances.

DIMACS CNF benchmarks are available for download from: `ftp://dimacs.rutgers.edu/pub/challenge/satisfiability/`.

6.4 Configure test

The previous chapter described a single execution of Molecular Simulation. Now we provide the automated invocation for processing datasets with each of the algorithms.

The provided Perl script `executeMolecularSat.pl` allows execution for a directory of DIMACS CNF input. Executing the script from the command line without arguments processes the experimental setup and saves output to the same directory.

```
$ perl executeMolecularSat.pl [options]
```

The options for `executeMolecularSat.pl` can be a combination of the options in Table 6.1.

Table 6.1: Command line options for `executeMolecularSat.pl`

Argument	**Parameters**	**Description**
`-d`		Distribution algorithm
`-l`		Lipton's algorithm
`-o`		Ogihara and Ray's algorithm
`-debug`		Debug
`-p`	`[CNF file path]`	Specify CNF file path. Default path: `data/testCNF`
`-f`		Write output to file

6.5 Execution and collection of data

The output can be analyzed after the automated tests have completed. The output consists of the standard SAT Competition output appended with custom runtime metric logging. We discuss viewing output directly during execution and reading saved output files. Collections of output files may be read by the data visualization program and exported into a condensed table.

6.5.1 Execution output

Molecular Simulation, by default, writes output to standard output on the console. With the `-f` option, output may be saved to a file. With the `-f` option specified, output gets saved with `[filename]-<a>.out`. The `[filename]` consists of the DIMACS CNF name and `<a>` specifies the algorithm type: `d`, `l` or `o`.

Output directed to standard output conforms to the SAT Competition rules. This output may be used during testing, or redirected to an external stream. The debug option `-debug` provides detailed information about the execution. The debug option writes verbose content based on the program execution.

Reading output metrics from the saved output, as defined in Table 5.2, allows for analysis of collected data. The data visualization reads a directory of output and condenses it as a `*.tsv` file. Subsequent datapoint browsing and the online view use the `*.tsv` file for condensed reading and transmission. In the next chapter, we provide the results of the experimental setup and discuss the design decisions for a general purpose molecular computer.

Chapter 7

Results

This chapter provides results of the k-Sat execution test from the previous chapter. We consider the results of the test and provide analysis of the algorithm metrics.

7.1 Algorithm metric comparison

This section provides results from the simulation. We provide the analysis for the molecular operations. These include counts of append, extract, mix, purify, splice, and split. Presentation of actual computation time and required memory for the solution representation allow for comparison of algorithms.

Append is an operation that concatenates molecules.

The Distribution algorithm is exponential in the number of appends. The operation count for append depends on the parsing order of the CNF expression.

Lipton's and Ogihara-Ray's algorithms use a fixed amount of appends. This depends on the number of variables and clauses present in the CNF expression.

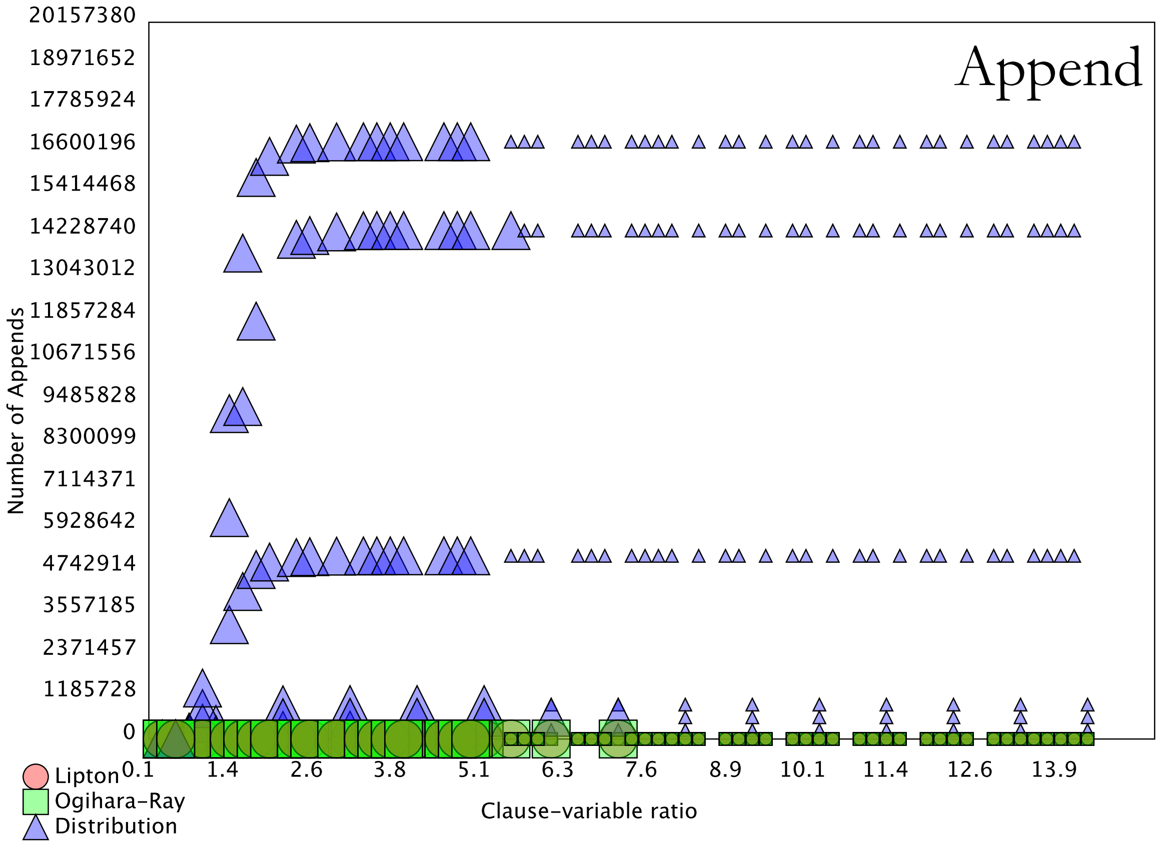

Figure 7.1: Clause to variable ratio α vs. Number of appends

Extract is an operation that filters strings.

Ogihara-Ray's algorithm requires the greatest amount of extracts. Lipton's algorithm is linear on α and varies a constant amount from Ogihara-Ray's algorithm.

The Distribution algorithm does not require extract.

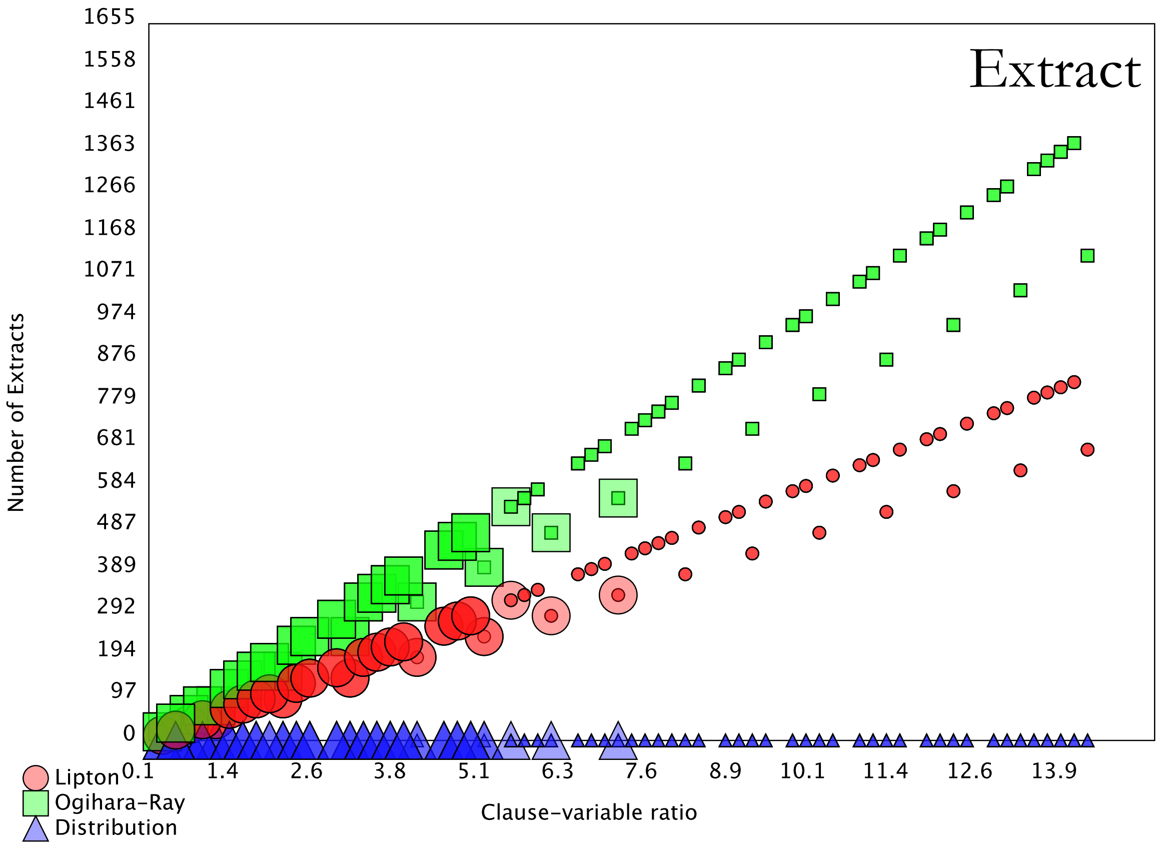

Figure 7.2: Clause to variable ratio α vs. Number of extracts

Mix is an operation that combines two tubes.

Lipton's algorithm requires a linear amount of mixes on α. The Distribution algorithm also requires a linear number of mixes, varying by a constant factor from Lipton's algorithm.

Ogihara-Ray's algorithm requires a constant amount of mixes on α.

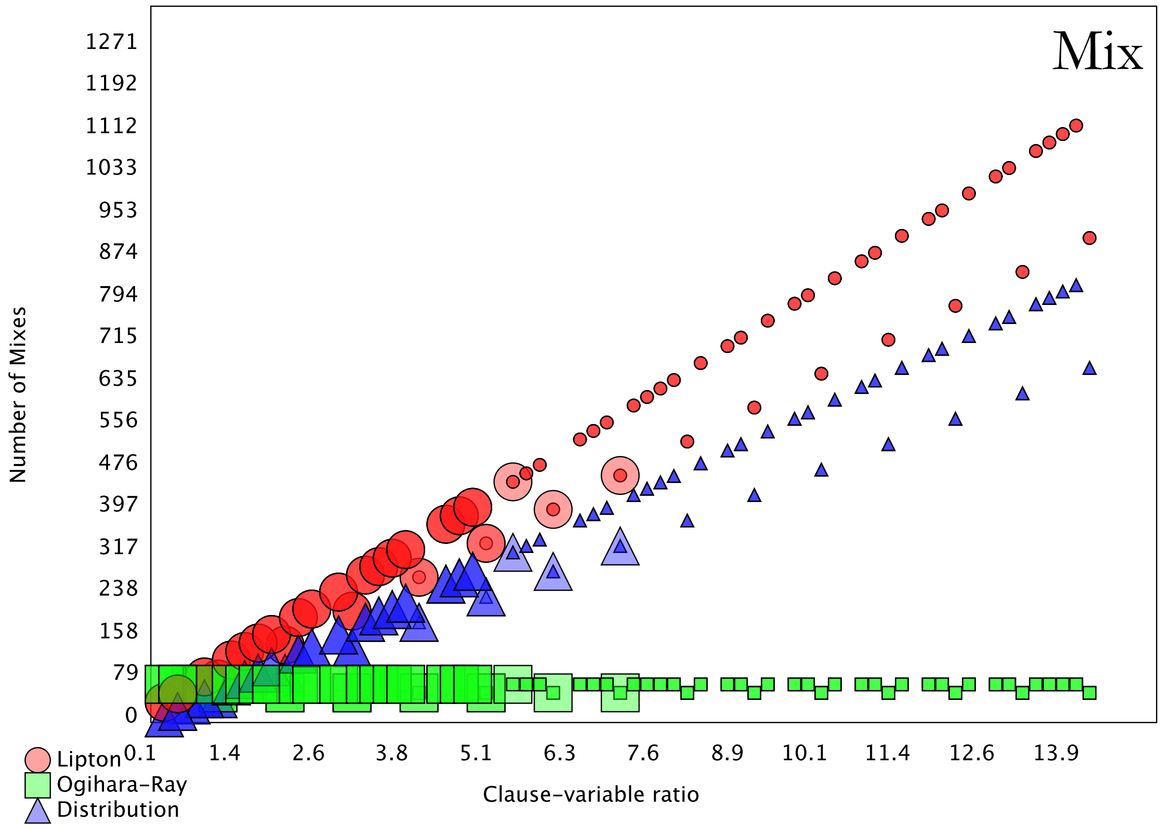

Figure 7.3: Clause to variable ratio α vs. Number of mixes

Purify is an operation that ensures equal portions of each independent string.

All three algorithms operate with a linear number of purifications on α. Ogihara-Ray's algorithm requires the greatest amount of purifications. The purifications vary by a constant amount when compared with Lipton's and the Distribution algorithms.

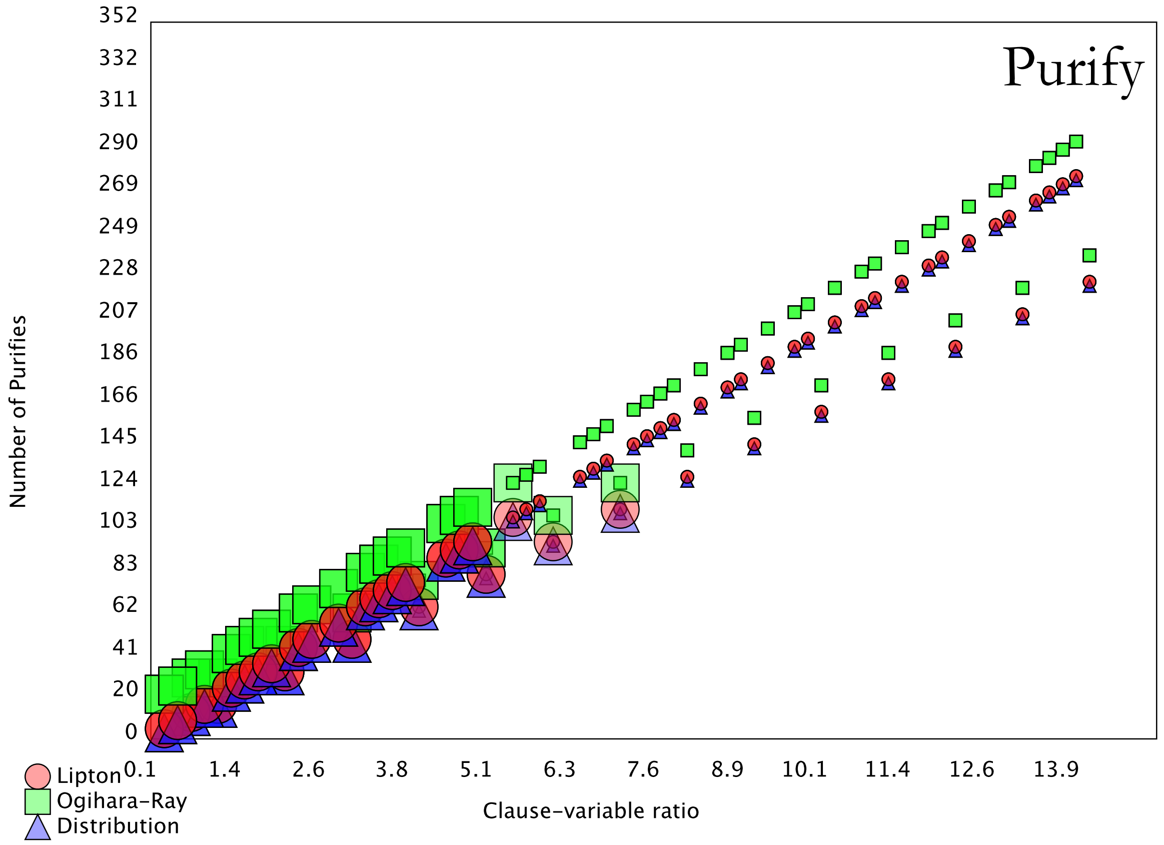

Figure 7.4: Clause to variable ratio α vs. Number of purifies

Splice is an operation that inserts a string at a targeted location.

The Distribution algorithm is exponential in the number of splices. The number of splices depends on the parsing order of the CNF expression. Each split requires reassembly, accomplished with two appends. Figure 7.1 shows the number of appends.

Lipton's and Ogihara-Ray's algorithms do not require splice the splice operator.

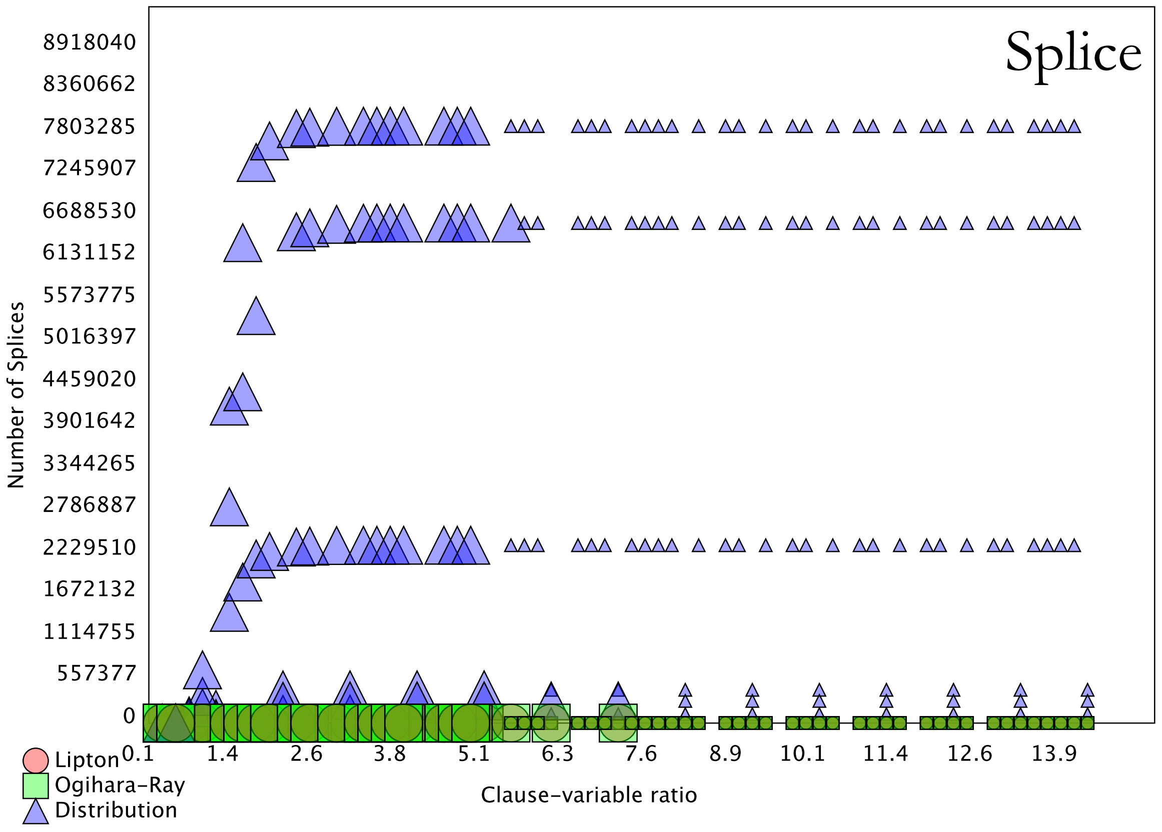

Figure 7.5: Clause to variable ratio α vs. Number of splices

Split is an operation that portions a tube into two exact copes.

Distribution requires a linear number of splits.

Lipton's and Ogihara-Ray's algorithms are constant in splits based the number of variables.

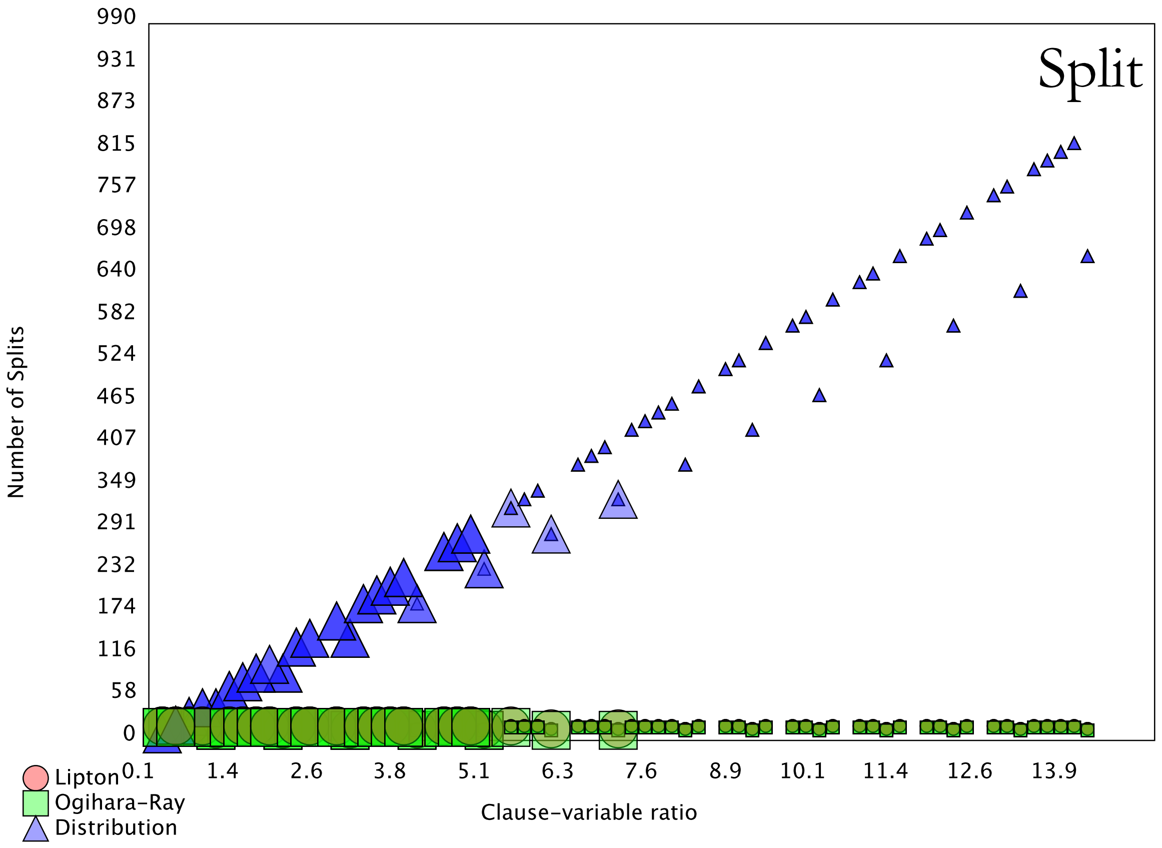

Figure 7.6: Clause to variable ratio α vs. Number of splits

Time is a measurement of algorithm execution in seconds.

Ogihara-Ray's algorithm requires the least amount of time. In cases where the SATISFIABILITY instance is under-constrained, where more possible solutions occur, the algorithm takes the greatest amount of time. Less pruning occurs in over-constrained instances, reducing the execution time of test instances.
Lipton's algorithm executes in exponential time with $\alpha \approx [4.2, 8.2]$ taking the longest. This is within the phase-transition region for 3-SAT.

The Distribution algorithm executes in exponential time, and performs better than Lipton's algorithm for low conflict ratios. However over the entire sweep performs worse than both Lipton's and Ogihara-Ray's algorithms. It shares the same $\alpha \approx [4.2, 8.2]$ during the 3-SAT phase-transition.

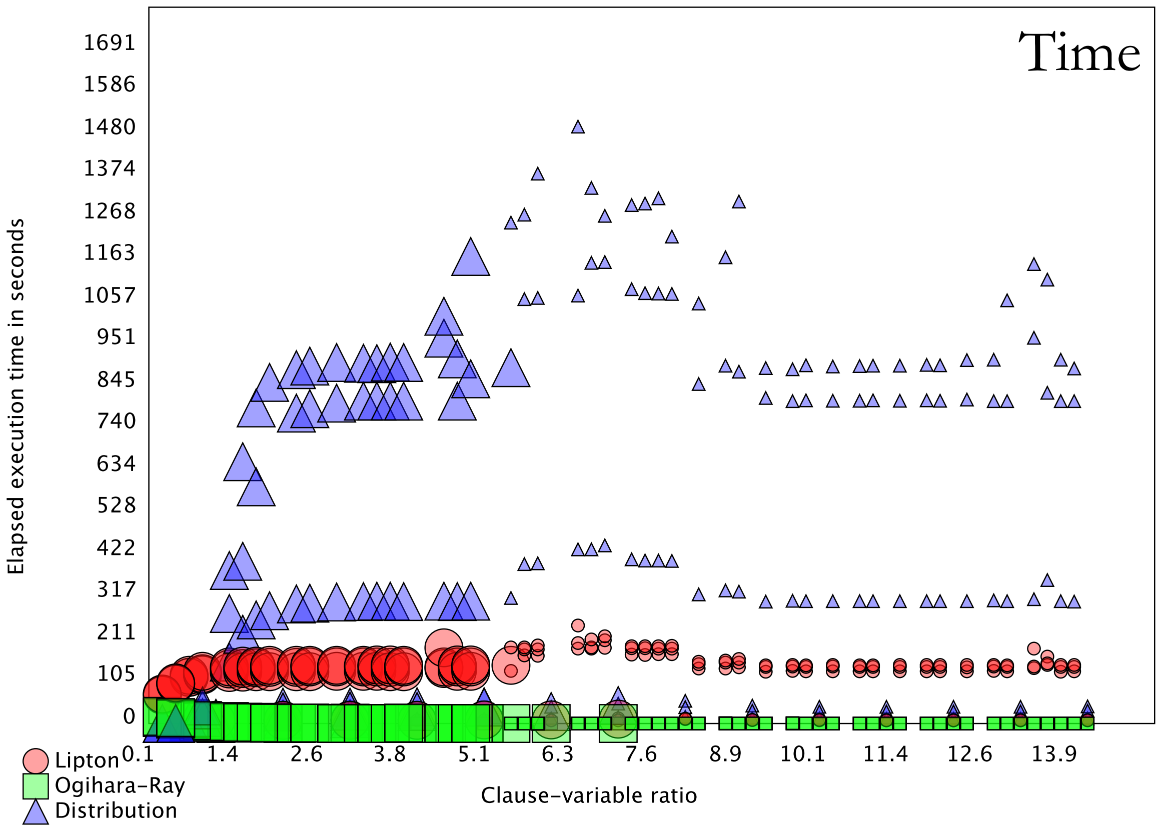

Figure 7.7: Clause to variable ratio α vs. execution time in seconds

Memory is a measurement of the satisfiable instance footprint returned by each algorithm measured in Bytes.

Lipton's and Ogihara-Ray's algorithms share the same solution footprint.

The Distribution algorithm contains a larger solution footprint after the trivially satisfiable instances with $\alpha \approx [0.2, 0.8]$. The space provides a set of non-conflicting assignments from $\alpha \approx [0.8, 2.9]$. Non-conflicting assignments consist of witnesses for only necessary variables.

Each SATISFIABILITY instance has a constrained solution space during the phase-transition region. All three algorithms share the same footprint. There are no satisfiable instances in this test with $\alpha > 7.2$. The axis in Figure 7.8 scales accordingly.

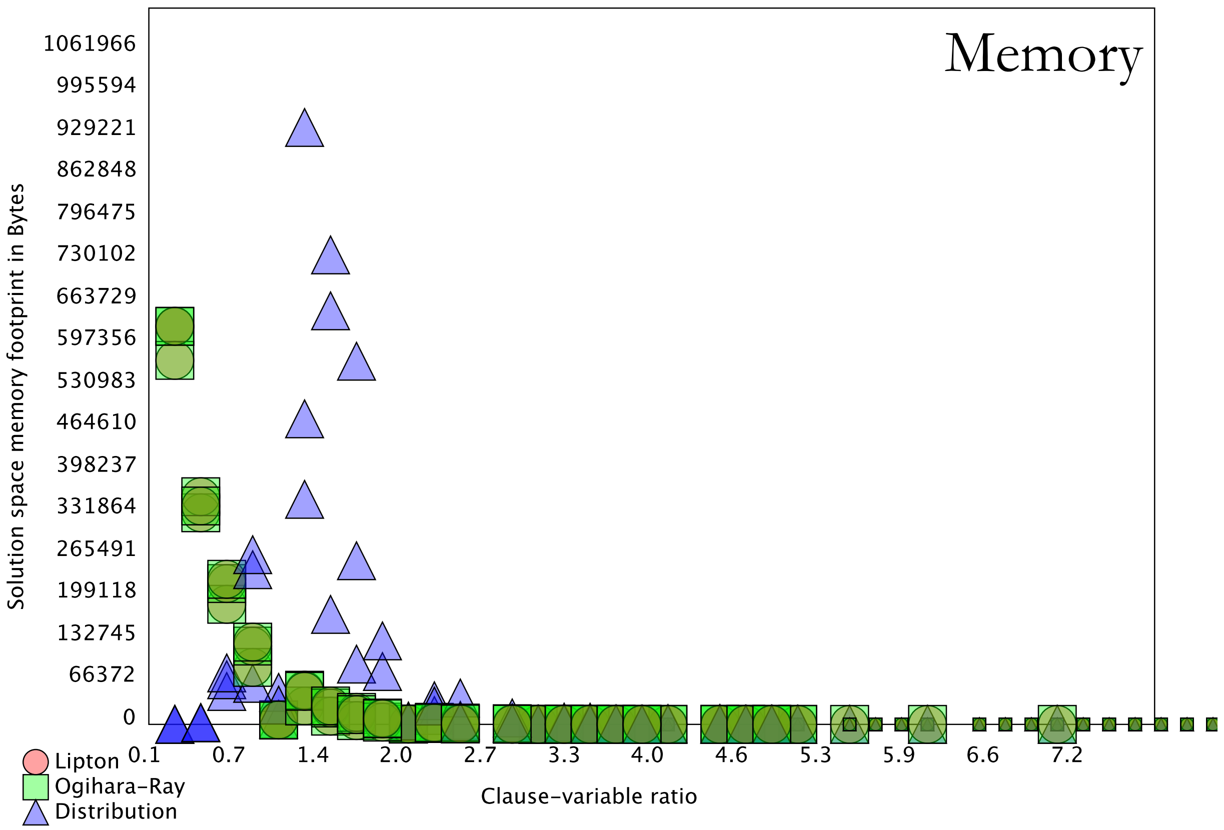

Figure 7.8: Clause to variable ratio α vs. satisfiable solution footprint in Bytes

Chapter 8

Conclusions

This project considered Satisfiability as a problem for general computation. We considered three molecular algorithms for Satisfiability and simulated their execution with a conventional computing implementation. In this chapter, we state the contributions of this project and directions molecular computation will take.

8.1 Contributions

We developed several contributions for molecular computing during this project. This includes introducing the molecular Distribution algorithm for Satisfiability in Chapter 4. We introduced Molecular Simulation in Chapter 5 and collected data from simulations of three molecular Satisfiability algorithms described in Chapter 6.

8.2 Future work

Nanopore sequencers have been designed for reading molecules and diagnosing patients in a medical setting. Extending the sequencing capability to a configurable molecular laboratory permits generalized computation.

Satisfiability provides a canonical input format for combinatorial problems. Molecular algorithms for Satisfiability may be constructed in gene sequencers designed as a configurable molecular laboratory.

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Appendix A

Source

A.1 Contributed

Download Molecular Simulation:

- `https://github.com/dncarley/MolecularSimulation`
- Documentation
  - Online Documentation:
    - `http://www.cs.rit.edu/~dnc6813/project/generatedDocs/index.html`
  - Offline Documentation:
    - `http://www.cs.rit.edu/~dnc6813/project/refman.pdf`

Download Sat Datapoints Visualization:

- `https://github.com/dncarley/VisualizeSatDatapoints`

A.2 External

Download David Wilson's *k*-Sat Generator:

- `http://research.microsoft.com/en-us/um/people/dbwilson/ksat/default.htm`

Download Doxygen:

- `http://www.stack.nl/~dimitri/doxygen/`

Download Ben Fry's examples for *Visualizing Data*:

- `http://benfry.com/writing/archives/3`

Appendix B

Molecular algorithm trace

B.1 Example Satisfiability instance

$$\phi = (x_1 \vee x_2 \vee \neg x_3) \wedge (x_2 \vee x_3 \vee \neg x_4) \wedge (\neg x_1 \vee \neg x_3 \vee \neg x_4)$$

B.2 Lipton's Algorithm

$$T = \textsc{Combinatorial Generate}(4)$$

$$T =$$

```
TTTT FTTT TFTT FFTT TTFT FTFT TFFT FFFT
TTTF FTTF TFTF FFTF TTFF FTFF TFFF FFFF
```

Next select Clause 1:

$$C_1 = (x_1 \vee x_2 \vee \neg x_3)$$

```
TTTT FTTT TFTT FFTT TTFT FTFT TFFT FFFT
TTTF FTTF TFTF FFTF TTFF FTFF TFFF FFFF
```

Extract x_1:

```
TTTT      TFTT      TTFT      TFFT
TTTF      TFTF      TTFF      TFFF
```

Extract x_2:

```
TTTT FTTT           TTFT FTFT
TTTF FTTF           TTFF FTFF
```

Extract $\neg x_3$:

```
                    TTFT FTFT TFFT FFFT
                    TTFF FTFF TFFF FFFF
```

Mix contents:

```
TTTT FTTT TFTT      TTFT FTFT TFFT FFFT
TTTF FTTF TFTF      TTFF FTFF TFFF FFFF
```

Next select Clause 2:

$$C_2 = (x_2 \vee x_3 \vee \neg x_4)$$

```
TTTT FTTT TFTT      TTFT FTFT TFFT FFFT
TTTF FTTF TFTF      TTFF FTFF TFFF FFFF
```

Extract x_2:

```
TTTT FTTT           TTFT FTFT
TTTF FTTF           TTFF FTFF
```

Extract x_3:

```
TTTT FTTT TFTT
TTTF FTTF TFTF
```

Extract $\neg x_4$:

```

TTTF FTTF TFTF      TTFF FTFF TFFF FFFF
```

Mix contents:

```
TTTT FTTT TFTT      TTFT FTFT
TTTF FTTF TFTF      TTFF FTFF TFFF FFFF
```

Finally, select Clause 3:

$$C_3 = (\neg x_1 \vee \neg x_3 \vee x_4)$$

```
TTTT FTTT TFTT      TTFT FTFT
TTTF FTTF TFTF      TTFF FTFF TFFF FFFF
```

Extract $\neg x_1$:

```
     FTTT                FTFT
     FTTF                FTFF      FFFF
```

Extract $\neg x_3$:

```
                    TTFT FTFT
                    TTFF FTFF TFFF FFFF
```

Extract x_4:

```
TTTT FTTT TFTT      TTFT FTFT
```

Mix contents:

```
TTTT FTTT TFTT      TTFT FTFT
     FTTF           TTFF FTFF TFFF FFFF
```

B.3 Ogihara and Ray's Algorithm

Initialize the tube T with initial vector assignments for variables x_1 and x_2

$$T = \{\texttt{TT}, \texttt{TF}, \texttt{FT}, \texttt{FF}\}$$

Iterate variable x_3:

$$C_1 = (x_1 \vee x_2 \vee \neg x_3)$$

$\neg x_3$ matches v_3

$$\begin{aligned} T_{P1} &= \{\texttt{TT}, \texttt{TF}\} \\ T_{N1} &= \{\texttt{FT}, \texttt{FF}\} \\ T_{P2} &= \{\texttt{FT}\} \\ T_P &= \{\texttt{TT}, \texttt{TF}, \texttt{FT}\} \end{aligned}$$

$$C_2 = (x_2 \vee x_3 \vee \neg x_4)$$

x_3 or $\neg x_3$ does not match v_3

$$C_3 = (\neg x_1 \vee \neg x_3 \vee x_4)$$

x_3 or $\neg x_3$ does not match v_3
Append

$$\begin{aligned} T_P &= \{\texttt{TTT}, \texttt{TFT}, \texttt{FTT}\} \\ T_N &= \{\texttt{TTF}, \texttt{TFF}, \texttt{FTF}, \texttt{FFF}\} \end{aligned}$$

Mix

$$T = \{\texttt{TTT}, \texttt{TFT}, \texttt{FTT}, \texttt{TTF}, \texttt{TFF}, \texttt{FTF}, \texttt{FFF}\}$$

Iterate variable x_4:

$$C_1 = (x_1 \vee x_2 \vee \neg x_3)$$

x_4 or $\neg x_4$ does not match v_3

$$C_2 = (x_2 \vee x_3 \vee \neg x_4)$$

$\neg x_4$ matchs v_3

$$\begin{aligned} T_{P1} &= \{\texttt{TTT}, \texttt{FTT}, \texttt{TTF}, \texttt{FTF}\} \\ T_{N1} &= \{\texttt{TFT}, \texttt{TFF}, \texttt{FFF}\} \\ T_{P2} &= \{\texttt{TFT}\} \\ T_P &= \{\texttt{TTT}, \texttt{FTT}, \texttt{TTF}, \texttt{FTF}, \texttt{TFT}\} \end{aligned}$$

$$C_3 = (\neg x_1 \vee \neg x_3 \vee x_4)$$

x_4 matches v_3

$$\begin{aligned} T_{P1} &= \{\texttt{FTT}, \texttt{FTF}, \texttt{FFF}\} \\ T_{N1} &= \{\texttt{TTT}, \texttt{TFT}, \texttt{TTF}, \texttt{TFF}\} \\ T_{P2} &= \{\texttt{TTF}, \texttt{TFF}\} \\ T_N &= \{\texttt{FTT}, \texttt{FTF}, \texttt{FFF}, \texttt{TTF}, \texttt{TFF}\} \end{aligned}$$

Append

$$\begin{aligned} T_P &= \{\texttt{TTT}, \texttt{TFT}, \texttt{FTT}\} \\ T_N &= \{\texttt{TTF}, \texttt{TFF}, \texttt{FTF}, \texttt{FFF}\} \end{aligned}$$

Mix

$$T = \{\texttt{TTT}, \texttt{TFT}, \texttt{FTT}, \texttt{TTF}, \texttt{TFF}, \texttt{FTF}, \texttt{FFF}\}$$

B.4 Distribution Algorithm

Initialize the tube T with the variables from the first clause

$$T = \{[1], [2], [-3]\}$$

Select Clause 2
  $T_1 = \textsc{InsertVariable}(T, 2)$

$$T_1 = \{[1, 2], [2], [2, -3]\}$$

  $T_2 = \textsc{InsertVariable}(T, 3)$

$$T_1 = \{[1, 3], [2, 3]\}$$

  $T_3 = \textsc{InsertVariable}(T, -4)$

$$T_3 = \{[1, -4], [2, -4], [-3, -4]\}$$

  $T = \text{mix}(T_1, T_2, T_3)$

$$T = \{[1, 2], [2], [2, -3], [1, 3], [2, 3], [1, -4], [2, -4], [-3, -4]\}$$

Select Clause 3
  $T_1 = \textsc{InsertVariable}(T, -1)$

$$T_1 = \{[-1, 2], [-1, 2, -3], [-1, 2, 3], [-1, 2, -4], [-1, -3, -4]\}$$

  $T_2 = \textsc{InsertVariable}(T, -3)$

$$T_2 = \{[1, 2, -3], [2, -3], [2, -3], [1, -3, -4], [2, -3, -4], [-3, -4]\}$$

  $T_2 = \textsc{InsertVariable}(T, 4)$

$$T_3 = \{[1, 2, 4], [2, 4], [2, -3, 4], [1, 3, 4], [2, 3, 4]\}$$

  $T = mix(T_1, T_2, T_3)$

$$\begin{aligned} T = \{&[-1, 2], [-1, 2, -3], [-1, 2, 3], [-1, 2, -4], [-1, -3, -4], \\ &[1, 2, -3], [2, -3], [1, -3, -4], [2, -3, -4], [-3, -4], \\ &[1, 2, 4], [2, 4], [2, -3, 4], [1, 3, 4], [2, 3, 4]\} \end{aligned}$$