Modular Arithmetic Expressions and Primality Testing via DNA Self-Assembly

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ABSTRACT. Self-assembly is a fundamental process by which supramolecular species form spontaneously from their components. This process is ubiquitous throughout the life chemistry and is central to biological information processing. Algorithms for solving many mathematical and computational problems via tile self assembly has been proposed by many researchers in the last decade. In particular tile set for doing basic arithmetic of two inputs have been given. In this work we give tile set for doing basic arithmetic (addition, subtraction, multiplication) of $n$ inputs and subsequently computing its modulo. We also present a tile set for primality testing. Finally we present a software ‘xtilemod’ for doing modular arithmetic. This simplifies the task of creating the input files to xgrow simulator for doing basic (addition, subtraction, multiplication and division) as well as modular arithmetic of $n$ inputs. Similar software for creating tile set for primality testing is also given.

Keywords: DNA self-assembly, error-correction, algorithmic self-assembly, Wang tile, DNA computing, Xgrow, XTile

1 Introduction

Self-assembly is a natural phenomenon observed at many places in nature such as formation of galaxies, formation of coral reefs, crystal growth etc. In 1996 Erik Winfree of California Institute of Technology, showed that it can be used to perform nano-scale computations [15]. This paved way for the birth of algorithmic self-assembly utilizing knowledge of three fields - DNA Nanotechnology [12] (due to the pioneering work of Ned Seeman in 1980s), DNA Computing (due to the pioneering work of L. Adleman in 1994) and Tiling Theory [13] (due to pioneering work of H. Wang who showed that zigsaw shaped colored tiles can simulate universal Turing machine). Winfree formulated the idea of molecular Wang tile using all this and showed that it can simulate universal Turing machine using abstract Tile Assembly Model (aTAM) [18, 8]. Algorithms for solving many mathematical and computational problems via tile self assembly has been proposed by many researchers in the last decade [6, 5, 4, 7]. The addition of two numbers with Wang tiles is given in the book [9]. In 2006 Brun [1, 2] gave algorithm for addition and multiplication of two numbers with...
aTAM and in 2008 Zhang and his coworkers [19] gave algorithm for subtraction and division of two numbers in aTAM. In this work, we extend the results and provide tile set for addition and multiplication of n numbers together with a tile set for arithmetic expression involving addition and subtraction. This is further extended to a tile set for modular arithmetic expression. Winfree's tile assembly model can be simulated using a program developed by him called Xgrow [17]. The input to Xgrow is a .tiles file. Many such standard .tiles files are distributed with the Xgrow package. In this paper, we also present a software package 'Xtilemod' for modular arithmetic that can be used to create such input files for the Xgrow simulator of Winfree by providing the basic arithmetic expressions. For further details on algorithmic self-assembly the reader is referred to excellent papers [16, 11, 10] and thesis [14, 5].

This paper is organized as follows. In Section 2, we give a brief overview of the aTAM. Section 3 provides the algorithms for addition and multiplication of n numbers via aTAM. Algorithm for arithmetic expression of n numbers involving addition and subtraction is described in Section 4 and algorithm for modular arithmetic expression of n numbers involving addition and subtraction is given in Section 5. Section 6 gives tile set for primality testing. In Section 7 we describe a software for modular arithmetic expressions which can produce the input to xgrow simulator. Finally Section 8 concludes the paper with some general remarks.

2 Background

Self assembly of DNA molecules can be approximated by mathematical models. Several such models have been given by many authors. In [18], Winfree gave a model called aTAM. The basic building block of a tile assembly model are square tiles. Each tile has 4 edges viz north, east, south and west with glues assigned to each edge. Each glue has some strength (usually an integer). Assembly starts with some seed tiles and frame tiles giving the initial input of the aTAM and a tile can attach to another tile if (1) the edges have matching glues and (2) the combined glue strength of both the tiles is greater than or equal to system temperature (again an integer, usually denoted by τ and we take τ = 2). Tiles can not be rotated. Under these settings system will grow from some initial tile set configuration to form a pattern or depending upon problem input it solves a problem. In Figure 1 a tile attaches to a seed configuration of 3 tiles. East glue a_1 of configuration tile and west glue of outside tile is of strength 2, all other tiles have glues of strength 1 except north of configuration tile and south of each tile in seed configuration that has strength 0. System temperature is τ = 2. It is shown by Winfree that such system is Turing universal. For more formal description the reader is referred to [3, 1, 2]. Recently basic arithmetic of two inputs with DNA Self Assembly have been studied by many authors [11, 2, 19]. In particular, two algorithms have been proposed by Brun [11, 2] for adding two numbers. Algorithm using L-configuration uses 16 computational tiles for addition whereas there is another economical tile set for adding two numbers which takes just 8 computational tiles. In [2], Brun also gave algorithm for multiplication of two numbers with 28 computational tiles. Algorithm for subtraction and division are given in [19]. In the next sections we will assume that the reader is familiar with the notations and definitions of [2, 19].
3 Basic Arithmetic of \( n \) inputs with DNA Self Assembly

3.1 Addition of \( n \) Numbers with 8 Computational Tiles

Suppose we want to add \( n \) positive integers \( \{a_1, a_2, \ldots, a_n | a_i \in \mathbb{Z}^+\} \). We can write their binary representation as \( a_j = \sum_{d=0}^{m_j} a_j^d 2^d \), where \( m_j = |a_j| \) is the size of the integer \( a_j \) and \( a_j^d \in \mathbb{Z}_2 \). If \( m = \max \{m_j | 1 \leq j \leq n\} \) then we can pad extra zeros to write \( a_j = \sum_{d=0}^{m} a_j^d 2^d \).

The next two Theorems gives the tile set for computing \( \sum_{i=1}^{n} a_i \).

Theorem 1. Let

\[
\Sigma_1 = \{s, t, 0, 1, 00, 01, 10, 11\} \cup \{#i | 1 \leq i \leq (m + n)(n - 2)\} \\
\cup \{$i | 1 \leq i \leq \max (m + n, 2n - 2)$\}
\]

be the set of glues and let \( T_1 \) be a set of tiles (different tiles types of \( T_1 \) are given in Table 1) over \( \Sigma_1 \) as described in Figure 2 then \( T_1 \) computes the function \( \sum_{i=1}^{n} a_i \).

The logic of the system is identical to a series of one-bit full adders. Each solution tile takes a bit from each of the inputs on the south side and a carry bit of the previous solution from the east side, and outputs the next carry bit on the west side and the sum on the north side. After computing the sum of two numbers, we need to combine this sum with next input bitwise. This process continues till all the integer inputs are added. To handle overflow we make size of each input \( a_i \) as \( n + m - 1 \) bits. We will illustrate it by an example.

Figure 3 shows a sample addition of \( 12 + 6 + 2 + 4 = 24 \) (\( m = 4, n = 4 \)). Input \( 12 = 1100_2 \) (size 4) and \( 6 = 110_2 \) (size 3) are given at the bottommost (first) row by adding extra zeros (to adjust overflow we make size of each \( n + m - 1 = 7 \) bits) and reading 12 from right side and 6 from left side. The sum is computed \( (12 + 6 = 18 = 10010_2) \) in second row and then passed to the 3rd row from left side, next input \( 2 = 10_2 \) is given from right side of 3rd row and the sum is computed in 4th row \( (12 + 6 + 2 = 20 = 10100_2) \) which is then passed to the 5th row from left side, next input \( 4 = 100_2 \) is given from right side of 5th row and the final sum \( 12 + 6 + 2 + 4 = 24 = 0011000_2 \) is computed in 6th row. Last row is added to stop the computation. Note that the example uses 5 left frame tiles, 4 corner tiles, 5 right frame tiles,
7 top frame tiles, 21 input tiles and 14 computational tiles (overall) matching the data given in Table 1.

Remarks: We have used 8 computational tiles in the algorithms, however we can optimize it a bit since the lower portion (10 or 01) of computational tiles gives same effect in computing the sum. Hence while implementing it in "xtilemod" (see Section 7) we have used 6 computational tiles.

Table 1: Total Tiles used for Computing $\sum_{i=1}^{n} a_i$ using 8 Computational Tiles

| Basic Tiles          | Tiles Types | Overall Tiles       |
|----------------------|-------------|---------------------|
| Left-Frame           | n-1         | 2n-3                |
| Corner               | 4           | 4                   |
| Right-Frame          | 2n-3        | 2n-3                |
| Top Frame            | 2           | n+m-1               |
| Input                | (2n-3)(n+m-1)| (n+m-1)(n-1)       |
| Computational        | 8           | (n+m-1)(n-2)        |

3.2 Addition of $n$ Numbers with $L$ type Tiles

**Theorem 2.** Let $\Sigma_2 = \{0,1,s,ss\} \cup \{\#i|1 \leq i \leq n + m - 1\} \cup \{\#c|0 \leq c \leq n\}$ and $T_2$ be a set of tiles (different tiles types of $T_2$ are given in Table 2) over $\Sigma_2$ as described in Figure 4. Then $T_2$ computes the function $\sum_{i=1}^{n} a_i$.

The logic of this system is similar to Theorem 2.2 of [2]. The tile set of addition of $n$ numbers using $L$ type tiles of [2] have been implemented in xtilemod (see Section 7).

Table 2: Total Tiles used for Computing $\sum_{i=1}^{n} a_i$ using $L$-type Computational Tiles

| Basic Tiles          | Tiles Types | Remark            |
|----------------------|-------------|-------------------|
| Left-Frame           | $1 + \sum_{k=2}^{n} m_k$ |                   |
| Right-Frame          | $\sum_{k=2}^{n} m_k$      |                   |
| Top Frame            | $2 + (n + m - 1)$        |                   |
| Computational        | Bruns' L-Type Tiles      |                   |

3.3 Multiplication of $n$ Numbers with Tiles

**Theorem 3.** Let $\Sigma_3 = \{0,1,00,01,10,11,20,21,\#\} \cup \{\#i|1 \leq i \leq nm - 2\} \cup \{\#j|nm \leq j \leq nm + (n - 1) + \sum_{k=2}^{n} m_k\}$ and $T_3$ be a set of tiles (different tiles types of $T_3$ are given in Table 3) over $\Sigma_3$ as described in Figure 5. Then $T_3$ computes the function $\prod_{i=1}^{n} a_i$.

Note that the size of $\prod_{i=1}^{n} a_i$ is $n + m$ bits, where $m = \max\{|m_j|1 \leq j \leq n\}$. WLOG, Suppose $a_1$ is of max size $m$. We put $a_1$ as an input at the bottommost horizontal base tiles and all other inputs are given in the vertical frame (right column) followed by a separator.
Figure 2: Tile Set for Computing \( \sum_{i=1}^{n} a_i \) using 8 Computational Tiles. Note that in Input Tiles (Figure 2(g) and 2(h)) each \( \alpha_{\theta}^j \in \mathbb{Z}_2 \) also \( a, b, c \in \{0, 1\} \).
tile. The idea of multiplication of \( n \) input integers is a simple extension of the Theorem 2.4 of [2]. The computational tiles also remain the same. The only difference is that \( n - 2 \) inputs are given in the vertical frame separated by one separator tile and subsequently one row. Figure 6 shows the product of \( 5 \times 4 \times 3 = 60 \). Note that the input \( 5 = 101_2 \) is given at the bottom row, input \( 4 = 100_2 \) is given as the first vertical input and \( 3 = 11_2 \) is given as second vertical input. The output is given at the top row as \( 60 = 111100_2 \).

Table 3: Total Tiles used for Computing \( \prod_{i=1}^{n} a_i \)

| Basic Tiles       | Tiles Types | Remark            |
|-------------------|-------------|-------------------|
| Horizontal-Frame  | \( 2(nm - 1) \) |                   |
| Seed              | 1           |                   |
| Vertical-Frame    | \( 2n + m_j \) |                   |
| Top Frame         | 6           |                   |
| Computational (including a copy tile) | 9 |   |

4 Arithmetic Expression of \( n \) Numbers with Addition and Subtraction: \( \sum_{i=1}^{n} \beta_i a_i, \ \beta_i \in \{+1, -1\} \)

**Theorem 4.** Let \( \Sigma_4 = \{0, 1, 00, 01, 10, 11, c_0, c_{-1}\} \cup \{d, e, f, g, h, l\} \) be the set of glues and let \( T_4 \) be a set of tiles (different tiles types of \( T_4 \) are given in Table 4) over \( \Sigma_4 \) as described in Figure 7. Then \( T_4 \) computes the function \( \sum_{i=1}^{n} \beta_i a_i, \ \beta_i \in \{+1, -1\} \).
(a) Typical Computational Tile

(b) All 8 Computational Tiles

(c) Top Frame Tiles

(d) Left Frame Tiles

(e) Input Frame Tiles

(f) Corner Tiles

(g) Example showing addition of $6 + 4 + 3 + 5 = 18$

Figure 4: Tile Set for Computing $\sum_{i=1}^{n} a_i$ using $L$ Type Computational Tiles. Note $a, b, c \in \mathbb{Z}_2$. 
Figure 5: Tiles set for Computing $\prod_{i=1}^{n} a_i$. Note $a, b, c \in \mathbb{Z}_2$.

Figure 6: Growth of Tiles for Computing the Product of $5 \times 4 \times 3 = 60$
The logic of the system is identical to a series of one-bit full adders or one bit subtractor depending on the operation which is to be performed. Each solution tile takes in a bit from each of the inputs on the south side and a carry bit from the previous solution tile on the east side, and outputs the next carry bit on the west side and the sum/subtracted value on the north side. In the subtraction the carry bit which is generated on the west indicates the requirement of 1 from the next left tile attached to it. For separating the operation of addition and subtraction + or - sign is attached in all the computational tiles on the east and the west side along with the computational bit. Due to this addition and subtraction can be done by just supplying the sign to computation from the right frame tile. We need to combine this result with next input bitwise. This process continues till all the integer inputs are operated. After operating it if output is positive then the same is displayed on the top row (which is the final output) but if output is negative then the output is converted into unsigned binary bit and this will be displayed on the top row (which is the final output) from the 2s complement. This is done because the normal output which was generated for negative value is in the 2s complement form. Also a negative sign is displayed with the negative result to tell the user that final output is negative. We will illustrate it by an example. Figure 8 shows a sample addition of \(6 - 12 + 4 - 2 = -4\). Input 6 = \(110_2\) and 12 = \(1100_2\) are given at the bottommost (first) row by adding extra zeros and reading 6 from right side and 12 from left side. The subtraction is computed \((6 - 12 = -6 = 11010_2)\) in second row and then passed to the 3rd row from left side, next input 4 = \(100_2\) is given from right side of 3rd row and the sum is computed in 4th row \((6 - 12 + 4 = -2 = 11110_2)\) which is then passed to the 5th row from left side, next input 2 = \(10_2\) is given from right side of 5th row and the final result \(6 - 12 + 4 - 2 = -4 = 1111100_2\) is computed in 6th row. Now as output is negative we have to convert it back into normal unsigned binary expression from 2s complement with a negative sign in front of it. To this the row 7th, 8th, 9th are used. Also the final result \(-0000100_2\) is printed on the 9th row.

| Table 4: Total Tiles used for Computing \(\sum_{i=1}^{n} \beta_i a_i, \ \beta_i \in \{+1, -1\}\) |
|--------------------------------------------------|
| Basic Tiles | Tiles Types | Remark |
| Left-Frame | 2n+5 | |
| Corner | 6 | |
| Right-Frame | 2n-1 | |
| Top Frame | 6 | |
| Input | (2n-2)(n+m-1) | |
| Computational (+) | 8 | |
| Computational (−) | 8 | |
| Other Computational | 4 | |
10

(a) Typical Computational Tiles for Addition, where
\[ \text{cout} = (a \land b) \lor (b \land c) \lor (c \land a) \]

(b) All 8 Computational Tiles for Addition

(c) Typical Computational Tiles for Subtraction (Refer Table 6)

(d) All 8 Computational Tiles for Subtraction

(e) Input Tiles for Bottom Row for Two Inputs \(1 \leq i \leq m + n - 1\)

(f) Intermediate Input Tiles (\(1 \leq i \leq n + m - 1\), \(3 \leq j \leq n\) and \(\lambda = i + (j-3)(n+m)\))

(g) Right Frame Tiles (\(ER: 1 \leq i \leq n - 1\)) and (\(SR: 1 \leq i \leq n - 2\)) and \(\lambda = 1 + (i - 1)(n + m), \beta^i \in \{+, -\}\) depending on position \(i\)

(h) Left Frame Tiles: \(1 < i < n - 2\), \(s \in \{C0, C1\}\)

(i) Top Frame Tiles

(j) Corner Tiles

(k) Other Computational Tiles

Figure 7: Tile Set for Computing \(\sum^n_{i=1} \beta_i a_i, \beta_i \in \{+1, -1\}\). Note \(a, b, c \in \mathbb{Z}_2\).
5 Modular Arithmetic Expression of \( n \) Numbers with Addition and Subtraction: \( \sum_{i=1}^{n} \beta_{i} a_{i}, \quad (\text{mod } t) \beta_{i} \in \{+1, -1\} \)

The tile set for computing \( \sum_{i=1}^{n} \beta_{i} a_{i}, \quad (\text{mod } t) \beta_{i} \in \{+1, -1\} \) is just an extended version of the \( \sum_{i=1}^{n} \beta_{i} a_{i}, \beta_{i} \in \{+1, -1\} \) tile set (See Theorem 4). We add tile set for division (from Lemma 2 of [19]) to the output of the \( \sum_{i=1}^{n} \beta_{i} a_{i}, \beta_{i} \in \{+1, -1\} \) tile set after ignoring sign bit. The final remainder of the output comes on the top most row. An example for \( 6 - 12 + 4 - 2 \pmod{3} = 1 \) is given in Figure 9. An implementation of the tile set is given in “xtilemod”.

6 Primality Testing with Tiles

**Theorem 5.** Let \( \Sigma_{5} = \{0, 1, 000, 001, 010, 011, 100, 101, 110, 111\} \cup \{=, 0, =, 1, 2, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, SS, RR, JJ, TT, WW, ZZ, KK, YY, XX, Y, K, X\} \) be the set of glues and let \( T_{6} \) be a set of tiles (different tiles types of \( T_{5} \) are given in Table 5) over \( \Sigma_{5} \) as described in Figure 10. Then \( T_{5} \) determines of primality of any input integer \( n \).

The logic of primality testing tile set is based on the Algorithm 1. We will illustrate it by an example. Figure 11 shows a sample primality testing for \( n = 5 = 101_{2} \). This binary input is given at the bottommost (first) row. These bits are copied to left side of the centre of each tile of 3 bits of second row. Second row also computes \( k = \lfloor \frac{n}{2} \rfloor \) and stores it in the right side of the centre of 3 bits of each tile. The middle bit out of these 3 bits on each tile centre in the second row is intermediate computation bit \( I \) (which is initially the bit of \( n \)). In fact
Figure 9: Example showing $6 - 12 + 4 - 2 = -4$ modulo 3
our input \( n \) always remain on left side in each row at the centre of each tile and the value of \( k \) remains same till \( I - k > 0 \) is true otherwise it changes to \( k - 1 \) and \( I \) becomes \( n \). Third row checks if \( k > 1 \), which is true in this case so we copy the content (all 3 bits) of centre of each tile to 4\(^{th} \) row (if \( k \) is not > 1 it quits and displays that it is not a prime). Next row 5\(^{th} \) checks if the content \( I \) corresponding to middle bit is > \( k \) (which is true) so \( I = I - k \) is done in 6\(^{th} \) row. Next row further checks if \( I - k > 0 \), which is true so we repeat previous step and \( I = I - k \) is done in 8\(^{th} \) row. Now 9\(^{th} \) row again checks if \( I - k > 0 \) which is not true this time so in 10\(^{th} \) row we do \( k = k - 1 \) and \( I = n \). In 11\(^{th} \) row again we check if \( k > 1 \) (just like 3\(^{rd} \) row) and we find that \( k = 1 \) so 12\(^{th} \) row gives the final output as 5 is prime.

**Algorithm 1 Primality Testing Algorithm**

| Require: \( n \) |
|------------------|
| Ensure: \( k = \left\lfloor \frac{n}{2} \right\rfloor \) |
| while \( k \neq 1 \) do |
| if \( n \mod k = 0 \) then |
| Not Prime |
| exit |
| else |
| \( k := k - 1 \) |
| end if |
| end while |

| Prime |

| Table 5: Total Tiles used for Primality Testing |
|-----------------------------------------------|
| Basic Tiles | Tiles Types | Remark |
| Left-Frame | 6 | |
| Corner | 6 | |
| Right-Frame | 10 | |
| Top Frame | 10 | |
| Input | \( n \) | |
| One bit to three bit converter | 4 | |
| Checking number > 1 | 12 | |
| Checking \( c > b \) | 24 | |
| Right to Left Moving without change | 4 | |
| Subtracting \( b - c \) | 16 | |
| Subtracting \( c - 1 \) | 16 | |

7 **Xtilemod: A Software Package for Modular Arithmetic Expressions**

Xtilemod is an modular arithmetic software package implemented in java which generates .tiles file according to options selected at runtime. For example if we have to add two num-
(a) Corner Tiles

(b) Top Frame Tiles

(c) Left Frame Tiles

(d) Right Frame Tiles

(e) Input Tiles

(f) Right to Left Move

(g) Subtracting $b - c$ Tiles (Refer Table 6)

(h) Subtracting $c - 1$ Tiles

(i) Checking $c > 1$

(j) Checking $c > b$ Out $\in \{=, <, >\}$ depending upon $b = c, b < c, b > c$

(k) One Bit to Three Bit Converter

Figure 10: Primality Testing. Note $a, b, c \in \{0, 1\}.$
Table 6: Subtraction Table Bitwise

| a | b | c | sum | cout | Figure 7(c) |
|---|---|---|-----|------|-------------|
| b | c | d | s | dout | Figure 10(g) |
| 1 | 1 | 1 | 1 | 1 | Figure 7(c) |
| 1 | 1 | 0 | 0 | 0 | Figure 10(g) |
| 1 | 0 | 1 | 0 | 1 | |
| 0 | 1 | 1 | 0 | 0 | |
| 0 | 1 | 0 | 1 | 0 | |
| 0 | 0 | 1 | 1 | 1 | |
| 0 | 0 | 0 | 0 | 0 | |

Figure 11: Primality Testing Example for $p = 5$
bers using 8 tile type addition then we will select the option 1 which chooses the operation of two numbers and thereafter option 1 of 1 which specifies 8-tile type addition. Last step to get the resultant tile design is to enter the input of integers. The code will display the name of file where the resultant output is loaded. For example if we are adding 6 and 12 using 8 tile type addition the output will be loaded in 
add_8_tile_12,6.tiles.
The resultant .tile file can be simulated using xgrow. The display will be binary. Red color of the resultant tile indicates 1 and the white indicates 0. Resultant tiles are generally at north with a few exception. In case of the division tile set the xgrow compilation displays the quotient at the west and the remainder at the north. In 8 tile addition of two numbers the output is shown at the middle and the inputs are both in the north and south direction. For more details the reader is referred to the user manual of the software available at [http://www.guptalab.org/xtilemod/manual.pdf](http://www.guptalab.org/xtilemod/manual.pdf). The tool ‘xtilemod’ is available for download at [http://www.guptalab.org/xtilemod](http://www.guptalab.org/xtilemod).

8 Conclusion

In this work we presented tile set for modular arithmetic expressions involving addition, subtraction, multiplication of \( n \) integers followed by a modulo operation and a software “xtilemod” for generating the corresponding .tiles files. A tile set for primality testing is also presented together with a java program “prime.java” for generating .tiles file. Due to space constraints we have omitted the proofs but the key ideas of each result are illustrated by examples, the detailed proof of the results will be reported in an extended version of the paper elsewhere.

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