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Power Analysis of an mRNA-Ribosome System

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ABSTRACT

Energy is the heart to drive any device, such as any machine. As researchers have been trying to perform low energy operations more and more, energy requirements are turning out to be one of the key features in measuring the performance of a device. On the other hand, as conventional silicon-based computing is approaching a barrier, needs of non-conventional computing is increasing. Though several such computing platforms have arisen to prove itself as a suitable alternative to silicon-based computing, less energy requirement is certainly one of the most sought features in the competition among the new platforms. Moreover, there are certain scenarios where performing calculations in pure bio-molecular ways are highly desired. Although DNA computing has already flagged the success of bio-molecular computing in terms of energy/power requirements, its manual nature keeps it behind from other computing techniques. Another new bio-molecular computing technique *Ribosomal Computing*, though still in infancy, has shown real promises due to its inherent automation. This work performs an analysis of the energy/power requirements of this computing technique. With the promising result obtained, ribosomal computing can claim itself as a promising computing technique, if combined with its inherent automation.

CCS CONCEPTS

• **Computing methodologies** → **Modeling methodologies**; **Model verification and validation**; • **Hardware** → *Biology-related information processing*;

KEYWORDS

Ribosomal Computing; mRNA-Ribosome System; Sequential Logic.

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1 INTRODUCTION

Silicon-based computing is about to face a major barrier due to several factors arisen from the miniaturization of transistors. At this moment of crisis in computing, several non-conventional computing techniques have emerged, such as *Quantum Computing*, *Bio-molecular computing* etc. Among these new computing techniques, bio-molecular computing has the advantage of less energy requirement. Moreover, there are certain scenarios such as implantable medical systems, as an example, drug delivery systems, would be much safer to be applicable if the electronic counterparts could be avoided. In such scenarios, a computing system made up purely of biological elements would be highly desirable.

Among the bio-molecular computing systems, current flag-holder DNA Computing has strong ability to solve computationally hard problems with ease. But huge manual interventions resist it from providing faster outputs when employed in solving general problems. To overcome this, a new bio-molecular computing Ribosomal computing has arisen that uses the automatic procedure of protein synthesis to perform the computations. This computing has already shown much promises via implementations of logic gates [4], sequential circuits [3] and shifter and comparator [2].

But any computing technique to prove itself promising should use as much low energy/power as possible. So, though ribosomal computing has shown its strength via inherent automation and has a clear win over DNA computing in this respect, to prove its real strength, it has to show that, ribosomal computing uses as much low energy/power as possible. This paper takes an attempt to show this added advantage of ribosomal computing and thus makes the ground of ribosomal computing excessively strong.

2 BACKGROUND

A cell, the basic unit of life, contains several cell structures, among which a ribosome molecule acts as a protein factory. After DNA (Deoxyribonucleic Acid) getting transcribed into mRNA (messenger Ribonucleic Acid), this cell structure translates the mRNA code into protein chain [14]. Amino acids, which are brought by tRNA (transfer RNA) on each successive reads of mRNA by the ribosome, are the basic units of a protein chain. In this section, at first, the basic structure of a ribosome molecule will be discussed followed by protein synthesis procedure. Along with protein synthesis procedure, various mutations form the basis of a mRNA-Ribosome computing system. Mutations followed by an overview of the workings of a mRNA-Ribosome system have been discussed following protein synthesis procedure.

2.1 Structure of a Ribosome

A ribosome molecule is a very tiny membrane-less cell structure and is composed of two subunits, *upper subunit*, and *lower subunit* [8]. Each subunit is composed of rRNA (ribosomal RNA) and protein molecules. rRNA can control the protein synthesis procedure[11].

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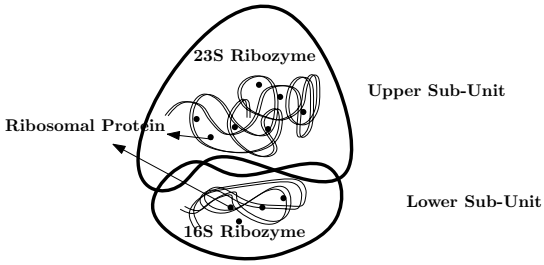

Figure 1: A ribosome molecule of prokaryotic cell [4]

Structural overview of a prokaryotic ribosome has been shown in figure 1.

A ribosome has three tRNA binding sites. *A site* selects and binds proper aminoacyl tRNA (tRNA with amino acid bound to its head) with the mRNA. In *P site* the amino acid is transferred to protein chain from the head of the tRNA. Through *E site* the empty tRNA exits from the ribosome. Other than these sites one nascent chain exit tunnel is present in a ribosome, through which final protein chain gets out of the ribosome. Ribosome also has a PTC (Peptidyl Transferase Center) that secretes *Peptidyl Transferase enzyme* to attach the newly arrived amino acid to the growing protein chain.

2.2 Protein synthesis Process

In protein synthesis process the genetic code in translated into protein chain [10]. A brief description of protein synthesis procedure is discussed as follows.

– At the starting of protein synthesis the mRNA is bound to lower subunit and the upper subunit gets attached to it to generate a complete mRNA-Ribosome System.

– Ribosome continues reading the mRNA triplet codons until *AUG* is read. It initiates protein synthesis procedure by bringing the tRNA having *Methionine* amino acid to *P site*.

– From the next codon read, proper tRNA binds to mRNA at *A site*. Then this tRNA gets a push by GTP (Guanosine Triphosphate). At that instant, PTC breaks the peptide bond between the tRNA present at *P site* and protein chain, and holds the chain. That tRNA of *P site*, which just lost its amino acid from its head goes to *E site*. Current aminoacyl tRNA that got push at *A site* comes to *P site*. The PTC releases the protein chain and attaches it to the new amino acid at the head of aminoacyl tRNA of *P site*. Again a new aminoacyl tRNA comes to *A site* depending on next triplet codon read at *A site* and protein synthesis continues in this manner until the stop codon is found.

– When stop codon is read at A site, no tRNA comes any further, protein synthesis stops, tRNA of *P site* loses the protein chain and exits via *E site*. Released protein chain comes out of the ribosome.

2.3 Mutations

A mutation is a biological process that changes the behavior of nucleotide base sequences by relocating, adding or deleting one or more nucleotide bases from the sequence. Suppressor mutation is a kind of mutation that can alleviate the effect of another mutation

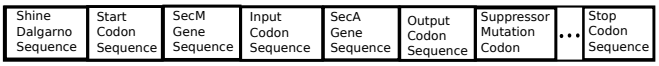

Figure 2: Reporter mRNA

[7]. Appropriate mutations in rRNA can affect the protein synthesis process.

2.4 An overview of Ribosomal Computing

Ribosomal computing deals with performing computations using mRNA-ribosome system with mutation in rRNA by following the protein synthesis process. The structure of the mRNA and required mutation varies from operation to operation. Detailed working of Ribosomal computing has been given in [4], [3], [2].

An example of ribosomal computing is implementation of logic gates as proposed in [4]. In logic gate implementation, the mRNA is designed from two n-bit inputs consisting of regions shown in figure 2 and briefly discussed as follows.

(1) First few nucleotide bases determine the Shine-Dalgarno sequence to identify the appropriate operating ribosome with suitably chosen mutations in rRNA.

(2) Start codon *AUG* to start protein synthesis.

(3) Then the two n-bit input numbers are represented by following main region containing n groups of gene sequences. Contents of each group are as follows.

– First sequence of a group is *SecM* gene sequence, that stalls protein synthesis.

– Corresponding bits from two inputs in bit interleaved fashion follows SecM. Each of two bits (0 and 1) are represented by specially chosen amino acids and corresponding triplet codons. This input codon sequence activates some particular mutation, if necessary.

– *SecA* gene sequence, that alleviates the stall and restarts protein synthesis, follows next.

– Two output bits (0 and 1) as output codon sequence follows SecA. A mutation can select one of these two codons to attach amino acid to output protein chain, and skip the other.

– Suppressor mutation to suppress currently activated mutation.

(4) Finally stop codon to stop the protein synthesis.

Appropriate ribosome molecule (having proper anti Shine-Dalgarno sequence and appropriate mutations) after obtaining the designed mRNA, outputs the desired protein chain automatically following its own natural course of protein synthesis procedure.

3 RELATED WORK

The fact that ribosome acts like a molecular machine has been shown by [11]. Various mathematical model of protein synthesis process has been simulated in [12]. The mathematical model of protein chain elongation is described in [6]. Even though various simulations via mathematical modelling of all aspects of ribosome and protein synthesis has ben proposed till date, simulation of artificial ribosome practically was not possible until 2015, when artificial ribosome using tethered subunit was implemented by [9]. Discovery of artificial ribosome led to the possibilities of performing computations using ribosome and automated process of protein synthesis

occurring within it. This artificial ribosome with reporter mRNA designed suitably to match the need of corresponding computation, is referred as *mRNA-Ribosome system*. This system has successfully been used to perform computations via the implementations of logic gates in [4], sequential circuits [3], and shifters and comparator [2].

4 POWER CALCULATION

The tRNA gets a push by the energy of GTP molecule as discussed in section 1. On the other hand, another GTP molecule is required for attaching a new amino acid to protein chain. Hence one GTP molecule is required if aminoacyl tRNA just passes through the ribosome without attaching any amino acid to the protein chain, and total of two GTP molecules are required if amino acid gets attached to the protein chain. Rest of the section shows the calculation of total energy/power requirement in terms of GTP molecules.

(1) SD sequence does not need any GTP molecule for processing.

(2) Start codon AUG requires two GTP molecules for processing, as Methionine amino acid gets attached in this read.

(3) In the following main region, n groups of codons are processed while operating on n bit numbers. Each of the regions, such as *SecM*, Input sequence, *SecA*, Output sequence and Suppressor Mutation requires various amount of GTP molecules for each of the n bits as follows.

Energy required for processing SecM : *SecM* attaches an amino acid to protein chain for each of its codon, and hence two GTP molecules are required for each. As a SecM protein contains *170* amino acids [1] [5], number of GTP molecules required is as follows.

$$E_{SecM}^{operation} = C_{SecM} \times 2 = 170 \times 2 \ = \ 340 \tag{1}$$

Energy required for processing SecA : Similar to SecM, SecA sequence needs two GTP molecule for processing each codon. As a SecA protein contains *901* amino acids, number of GTP molecules required is as follows.

$$E_{SecA}^{operation} = C_{SecA} \times 2 = 901 \times 2 \ = \ 1802 \tag{2}$$

Energy required for processing input sequence : If input sequence is enclosed between SecM and SecA, then no amino acid will be attached to protein chain and one GTP molecule will be required for each codon. Otherwise, as in shifters, where no SecM or SecA sequence is used, two GTP molecules are required for each input codon. If C_{ip} be total number of input codons for each bit information, then number of GTP molecules required is as follows.

$$E_{ip}^{operation} = C_{ip} \times \alpha \tag{3}$$

, where α is 1 (if no amino acid gets attached due to input sequence), or 2 (otherwise).

Energy required for processing output sequence : Output codon may be or may not be selected. If some particular codon is selected then two GTP molecules are required as amino acid is attached to protein chain. Otherwise one GTP molecule is required. Let us assume C_{op_1} be the number of selected codons and C_{op_2} be the number of skipped codons. Required number of GTP molecules then is as follows.

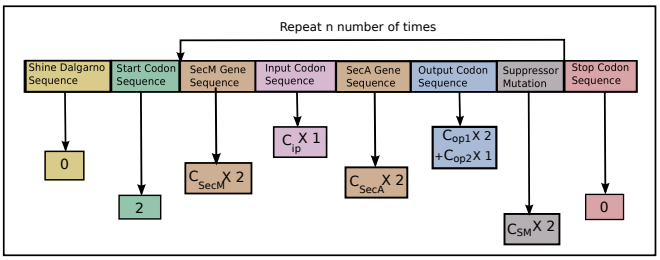

Figure 3: GTP calculation for mRNA of Logic gate Ribosome

$$E_{op}^{operation} = C_{op_1} \times 2 + C_{op_2} \times 1 \tag{4}$$

Energy required for processing suppressor mutation : For suppressor mutation two cases may occur depending on its position. If it is enclosed within SecM and SecA along with input sequence, as required in implementation of sequential circuit, no amino acid gets attached due to it and single GTP molecule is required. Otherwise it resides after output sequence, thus outside of region enclosed within SecM and SecA, and hence two GTP molecules are required. So, number of GTP molecules required will be as follows.

$$E_{SM}^{operation} = C_{SM} \times \beta \tag{5}$$

, where C_{SM} is the number of codons present in suppressor mutation, and β is 1 (in case of sequential circuit), or 2 (otherwise).

(4) After processing the main region comes the stop codon, that stops the protein synthesis procedure. This region does not require any GTP molecule to process.

Total number of GTP molecules required to supply energy for an n bit operation in a mRNA-Ribosome system can then described as in equation 6.

$$E_{n_{total}}^{operation} = 2 + n \times (340 + 1802 + E_{ip}^{operation} + E_{op}^{operation} + E_{SM}^{operation}) \tag{6}$$

The energy requirement for SD sequence, start codon and stop codon is similar for each operation. The energy required for performing the main region may only get varied. So, the energy required for main region for all the operations are shown in rest of the sections.

4.1 GTP Requirement Calculation for Boolean Logic Operation

The GTP requirement for each step of mRNA for boolean logic operation is given in the figure 3.

4.1.1 Example of GTP Requirement Calculation for XOR gate. Energy requirement for performing the XOR on the main region of mRNA in figure 3 is calculated as follows.

(1) Number of GTP molecules required to perform SecM operation according to equation 1 is 340.

(2) The number of GTP molecules required to process input sequence according to equation 3 is as follows, as each group of input codon sequence consists of two triplet codons.

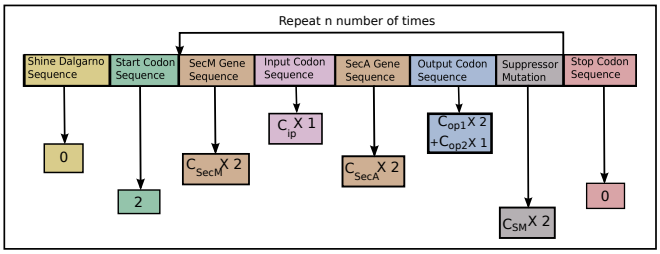

Figure 4: GTP calculation for mRNA of Comparator Ribosome

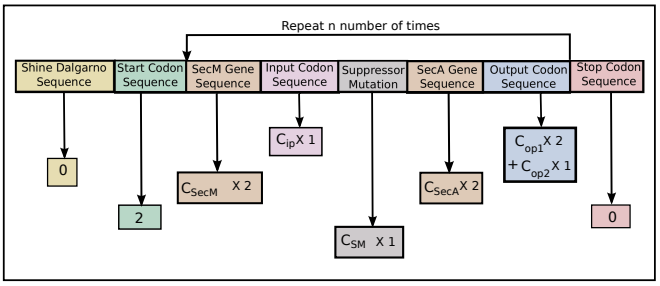

Figure 5: GTP calculation for mRNA of sequential circuit

$$E_{ip}^{xor} = C_{ip} \times 1 = 2 \times 1 = 2$$

(3) Number of GTP molecules required to perform SecA operation according to equation 2 is 1802.

(4) Two output codons are present after output sequence, one of which is selected and the other one is skipped. The number of GTP molecules required for processing the output sequence according to equation 4 is as follows.

$$E_{op}^{xor} = C_{op_1} \times 2 + C_{op_2} \times 1 = 1 \times 2 + 1 \times 1 = 3$$

(5) We consider here that the suppressor mutation for XOR gate consists of 2 sense codons (nonsense codons may also be present in general in an mRNA molecule, which do not attach any amino acid). So, GTP molecules required to process the suppressor mutation is as follows according to equation 5.

$$E_{SM}^{xor} = C_{SM} \times 2 = 2 \times 2 = 4$$

To process each bit information of mRNA 3 main region, number of GTP molecules required is $340 + 2 + 1802 + 3 + 4 = 2151$. So, to perform logic operation on n bit inputs, number of GTP molecule required is $2 + (2151 \times n)$.

4.2 GTP Requirement Calculation for Comparator Logic Operation

The GTP requirement for each step of of mRNA for comparator logic operation is shown in the figure 4.

4.2.1 Example of GTP Requirement Calculation for Comparator logic. Energy requirement for processing the main region while performing the comparator operation on mRNA of figure 4 is calculated as follows.

(1) Number of GTP molecules required to perform SecM operation according to equation 1 is 340.

(2) The number of GTP molecules required to process input sequence according to equation 3 is as follows, as two inputs are involved in a comparator operation.

$$E_{ip}^{comparator} = C_{ip} \times 1 = 2 \times 1 = 2$$

(3) Number of GTP molecules required to perform SecA operation according to equation 2 is 1802.

(4) In comparator mRNA, three output codons are present in each group of output sequence. Among them one will be selected at a time, and the rest of the two will be skipped. The number of GTP molecules required for processing the output sequence according to equation 4 is as follows.

$$E_{op}^{comparator} = C_{op_1} \times 2 + C_{op_2} \times 1 = 1 \times 2 + 2 \times 1 = 4$$

(5) Here we consider that the suppressor mutation sequence consists of 2 sense codons. The number of GTP molecules required to process the suppressor mutation sequence according to equation 5 is as follows.

$$E_{SM}^{comparator} = C_{SM} \times 2 = 2 \times 2 = 4$$

So, $340 + 2 + 1802 + 4 + 4 = 2152$ GTP molecules is required for each bit of mRNA 4 main region in comparator operation. So, to perform comparison on n bit inputs, number of GTP molecule required is $2 + (2152 \times n)$.

4.3 GTP Requirement Calculation for Sequential Circuit

The GTP requirement for each step of mRNA for sequential logic operation is given in the figure 5, that in fact represents the mRNA structure for JK flip-flop operation [3].

4.3.1 GTP Requirement Calculation for JK flip-flop. Energy requirement for performing JK flip flop operation on mRNA of figure 5 is calculated as follows.

(1) Number of GTP molecules required to perform SecM operation according to equation 1 is 340.

(2) The number of GTP molecules required to access input codon according to equation 3 is as follows.

$$E_{ip}^{Flipflop} = C_{ip} \times 1 = 2 \times 1 = 2$$

(3) Assuming similarly that, JK Flip-flop requires two codons for suppressor mutation, number of GTP molecules required for processing the suppressor mutation is as follows.

$$E_{SM}^{Flipflop} = C_{SM} \times 1 = 2 \times 1 = 2$$

, as the suppressor mutations, being within SecM and SecA, do not attach any amino acid.

(4) Number of GTP molecules required to perform SecA operation according to equation 2 is 1802.

(5) Two output codons are required, one of which is selected and the other one is skipped. So, the number of GTP molecules required to process the output codon sequence is as follows.

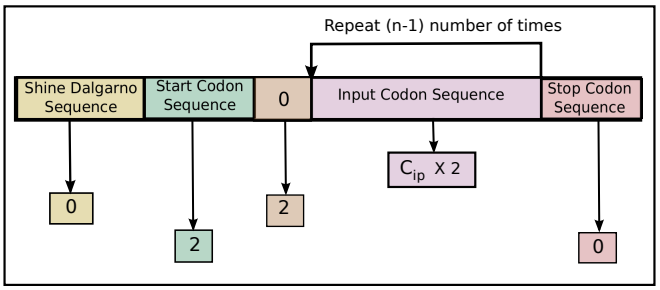

Figure 6: GTP calculation for mRNA of Logical Right Shift

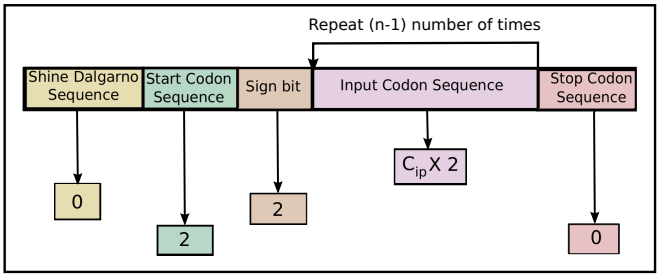

Figure 7: GTP calculation for mRNA of Arithmetic Right Shift

$$E_{op}^{Flopflop} = C_{op_1} \times 2 + C_{op_2} \times 1$$
$$= 1 \times 2 + 1 \times 1 = 3$$

So, $340 + 2 + 2 + 1802 + 3 = 2149$ GTP molecules are required for each bit of main region of mRNA in JK flip flop operation. So, to perform flip flop operation on n bit inputs, number of GTP molecule required is $2 + (2149 \times n)$.

4.4 GTP Requirement Calculation for Shifters

4.4.1 Logical Right Shift. Energy requirement for processing the main region of mRNA of figure 6 to perform logical right shift operation on an n-bit number is calculated as follows.

(1) Triplet codon corresponding to *0* is attached at the beginning of main region to have it attached as the prefix of output protein chain. To process it, 2 GTP molecules are required.

(2) For each of the rest of $(n-1)$ bits, number of GTP molecules required to process is as follows.

$$E_{ip}^{LRS} = C_{ip} \times 2 = 1 \times 2 = 2$$

So, to perform logical shifting on n bit inputs, number of GTP molecules required is $2 + (2 + 2 \times (n-1)) = 2 + 2 \times n$.

4.4.2 Arithmetic Right Shift. Energy requirement for processing the main region of mRNA of figure 7 to perform arithmetic right shift operation on an n-bit number is calculated as follows.

(1) Triplet codon corresponding to sign bit is attached at the beginning of main region to have it attached as the prefix of output protein chain. To process it, 2 GTP molecules are required.

(2) For each of the rest of $(n-1)$ bits, number of GTP molecules required to process is as follows.

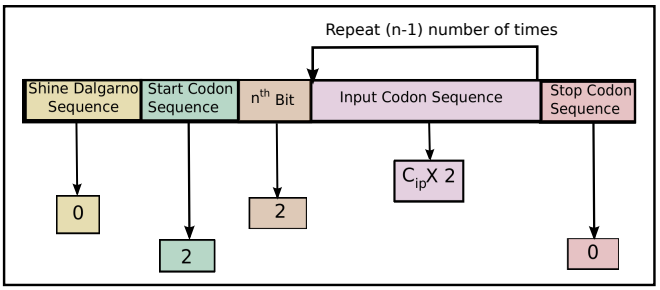

Figure 8: GTP calculation for mRNA of Circular Right Shift

$$E_{ip}^{ARS} = C_{ip} \times 2 = 1 \times 2 = 2$$

So, to perform logical shifting on n bit inputs, number of GTP molecules required is $2 + (2 + 2 \times (n-1)) = 2 + 2 \times n$.

4.4.3 Circular Right Shift. Energy requirement for processing the main region of mRNA of figure 8 to perform logical right shift operation on an n-bit number is calculated as follows.

(1) Triplet codon corresponding to n^{th} bit is attached at the beginning of main region to have it attached as the prefix of output protein chain. To process it, 2 GTP molecules are required.

(2) For each of the rest of $(n-1)$ bits, number of GTP molecules required to process is as follows.

$$E_{ip}^{CRS} = C_{ip} \times 2 = 1 \times 2 = 2$$

So, to perform logical shifting on n bit inputs, number of GTP molecules required is $2 + (2 + 2 \times (n-1)) = 2 + 2 \times n$.

4.5 Power dissipation by GTP hydrolysis

In GTP hydrolysis a phosphate bond of a GTP molecule is broken and a phosphate molecule is released with some energy. After this hydrolysis, GTP becomes GDP (Guanosine Diphosphate). Amount of energy released in this operation is 4.3 $kcal/mole$ or 17.99 $kilo-joule/mole$. One mole signifies *Avogadro's number* of atoms in unit volume and that is $6.022140857 \times 10^{23}$. On the other hand, in one second, 20 amino acids are processed, requiring 40 GTP molecules on average. So, total power dissipation from a GTP hydrolysis can be obtained as follows.

$$\frac{17.99 \times 10^3 \times 40}{6.023 \times 10^{23}} J/s = 1.1947 \times 10^{-18} J/s \quad (7)$$

4.6 Discussion

4.6.1 Power requirements of Logic Gates due to GTP hydrolysis. According to equation 7, the amount of dissipated power from GTP hydrolysis involving *40* GTP molecules per second is 1.1947×10^{-18} J/s. $2151 + 2 = 2153$ number of GTP molecules are required to perform single bit XOR operation. So total power dissipated for hydrolysis of 2153 GTP molecules will be as follows.

$$\frac{2153 \times 1.1947 \times 10^{-18}}{40} = 6.4305 \times 10^{-17} J/s$$

Table 1: Comparative power calculations of an mRNA-Ribosome system with conventional machine for different logic units.

Name of operation	Power requirement in conventional machine	Power requirement in mRNA-Ribosome System
XOR	4.2×10^{-8}	6.4305×10^{-17}
Comparator	2.1×10^{-7}	6.4335×10^{-17}
Flip Flop	1.68×10^{-7}	6.4245×10^{-17}
Shifter	1.68×10^{-7}	1.1947×10^{-19}

But even in the latest and best CMOS technology, FinFET technology, a XOR operation dissipates the power of 4.2×10^{-8} J/s to perform XOR operation [13].

4.6.2 Power requirements of Comparator operation due to GTP hydrolysis. The number of GTP molecules required to perform a single bit comparison is $2152+2 = 2154$. So, the power dissipation for hydrolysis of 2154 GTP molecules is given in equation 4.6.2.

$$\frac{2154 \times 1.1947 \times 10^{-18}}{40} = 6.4335 \times 10^{-17} J/s$$

In FinFET technology, assuming all gates consume same amount of power, a comparator, containing *5* gates, dissipates the power of $4.2 \times 10^{-8} \times 5 = 2.1 \times 10^{-7}$ J/s to perform the operation [13].

4.6.3 Power requirements of Sequential circuit due to GTP hydrolysis. The number of GTP molecules for a single bit flip flop operation is $2149 + 2 = 2151$. So, the power dissipation for hydrolysis of 2151 GTP molecules is given in equation 4.6.4

$$\frac{2151 \times 1.1947 \times 10^{-18}}{40} = 6.4245 \times 10^{-17}$$

In FinFET technology, a sequential circuit, such as JK flip-flop, containing *4* gates, dissipates the power of $4.2 \times 10^{-8} \times 4 = 1.68 \times 10^{-7}$ J/s to perform the operation [13].

4.6.4 Power requirements of Shifter operation due to GTP hydrolysis. The number of GTP molecules required to perform a single bit shifter operation is $2 + 2 = 4$. So, the power dissipation for hydrolysis of 4 GTP molecules is given in the equation 4.6.4

$$\frac{4 \times 1.1947 \times 10^{-18}}{40} = 1.1947 \times 10^{-19}$$

In FinFET technology, a shifter, such as a single bit shift register, being composed of single flip-flop, also dissipates the power of 1.68×10^{-7} joule in one second to perform the operation [13].

Table 1 provides a comparative view of power requirements for the discussed important operations on a conventional machine and on an mRNA-Ribosome system.

5 CONCLUSION

Energy requirements is one of the major factors in determining the efficiency and performance of any machine, such as any computational device. As the conventional computing is approaching a barrier, more and more non-conventional computing techniques are coming in front. Newest addition to this field is a bio-molecular computing referred as Ribosomal computing. Though DNA computing is a very promising non-conventional computing technique, it lacks automation. Ribosomal computing arose to answer that crisis and to provide automation in computation using bio-molecular techniques. Though [4], [3] and [2] prove this possibility of automation, but to make the ground really strong it was needed to be proved that it needs very less energy in doing the job. This work does the same and thus makes the ground of Ribosomal computing strong enough to prove itself as a powerful non-conventional computing technology.

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