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Analysing the Parallel Scalability of Mechanical Nano-computers Through Interconnection Network Evaluators for Pharmaceutical Applications

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Abstract

This paper explores the potential of mechanical nano-machines for computation by evaluating its parallelisation power through static interconnection network evaluations. It investigates the mechanical nano-machine model as a 2-Dimensional mesh to analyse factors like diameter, bisection width, arc connectivity, and cost. The research suggests that around 448 nanogears per machine offers an ideal balance between minimizing diameter and bisection width while maximizing connectivity, proving that a mechanical nano-computer is indeed parallelisable. This highlights the potential scalability of mechanical nano-computers, showcasing their potential in pharmaceutical applications.

Keywords: Nano-computers**,** Interconnection network evaluation, Pharmaceutical applications, Nanotechnology.

1. Introduction

Since its conceptual birth in the 1950s, nanotechnology has come a long way. The modelling and development of nano-machines have resulted in a significant shift in the way we view nano-technology. At present, science recognizes various types of nano-machines (machines that use components of a nano-scale, or a scale of one billionth of a meter, or 10^{-9} meters, and perform various computational tasks as machines do) which have all been documented as a result of relentless research in the nano-realm.

One of such machines are the Molecular Nano-machines (or nano-technology), which come under the umbrella of Mechanical Nano-computers. Introduced by K. Eric Drexler in 1987 (Drexler et al., 1987), the broader vision of Molecular Nano-technology (MNT) that consisted of the brand new ‘mechanical nanomachines’ largely served as a foundation for a new nano-technological model. At a molecular level, nano-machines, being a class of machines that are so small in scale yet can respond to inducements with mechanical movements (that of switches, gears, and motors), find their potential way into various fields of modern research and design of mechanical computing devices, while still being in the process of development and improvement (Wang et al., 2009). The Drexler model comprises of rods and bumps with tiny mobile components called nanogears that encode information. As a whole, a molecular or mechanical nano-machine was proposed to resemble a graph of strongly connected components, or a nano-scale network model.

Mechanical machines, in summary, replace electronic components with mechanical work to perform computations. Combining this with nano-machines, we aim to understand the mechanical computation power of nano-

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computers at various levels. This paper this discusses the behaviour of mechanical nano-machines as a network model, applying mathematical evaluation equations to determine the cost, connectivity, bisection, and diameter of these mechanical nano-networks. This will provide us with useful data that can help in calculating the computing power as parallel entities, cost, and optimisation of mechanical nano-computers, finding their worth in the future of nano-science and parallel computing. Finally the scalability (increasing components while obtaining viable results) of the mechanical nano-machines can also be assessed.

The paper is organised as follows: Related Work in Section II gives insight into the root of this research, the Research Methodology discussing the inferences on these mechanical nano-machines, while sections IV, V and VI confer the Implementation Details, Results Inferred, and Conclusion along with Future Implementations, respectively.

2. Related Work

Although the research and development of mechanical computing nano-machines have been limited and relatively new, the vision of Drexler to create nano-machines that can perform complex computation has been closer than ever. The computation power of mechanical nano-machines has exponentially increased on paper as the optimization of gates, levers, gears, switches, and springs was prioritized, with its usability and innovation surpassing boundaries that were inconceivable in 1986, when the research for nanotechnology and nano-machines was still in its nascent stages. At present, the Moore's law bottle neck and other such obstacles have been overcome by scientific advancement and configuration of nano-mechanical components (Way et al., 2010).

2.1. Structure of Drexler's Model

Drexler's proposed model consisted of node-like nanogears that perform the primary task of data and information encoding. These gears would roll around the others to create the calculation and data transfer among different nano-machines. The rods would intersect and connect the nodes within that nano-machine together. The calculation that takes place through rolling and ticking of the nanogears is similar to the model of a Pascaline computational device. If looked at it in another perspective, when flattened, these nano-machines form a mesh of gears and rods (Buell et al., 1973). Therefore, the mechanical nano-computer model introduced by Drexler can be assumed to be a 2-Dimensional mesh with wraparound for the sake of mathematical calculations. Farhat et. al. introduced a mathematical model to analyse the connectivity and its shape in a 2-Dimensional mesh with wraparound and without wraparound (Buell et al., 1973).

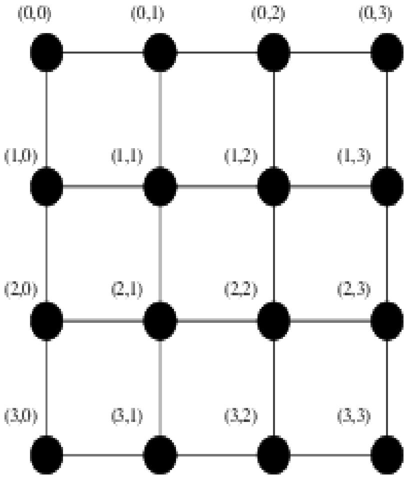


Figure 1 The 2-Dimensional mesh without wraparound for n ∈ {4}.

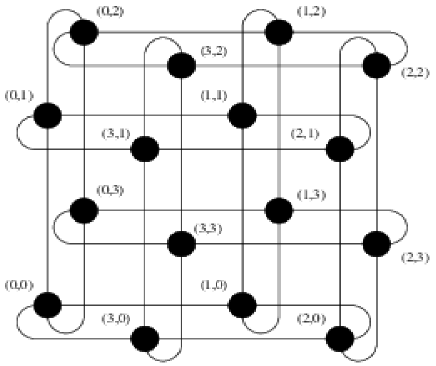


Figure 2 The 2-Dimensional mesh with wraparound for n ∈ {4}.

2.2. Limitations of the Drexler Model

The Drexler-Smalley debate argued the material limitations of the Drexler MNT model (Johnson et al., 2007). Smalley questioned the feasibility of constructing assemblers that work on a molecular level. However, the scalability potential of the mechanical nano-computers still appear remarkable at a conceptual level.

This model of a n-dimensional 2-Dimensional mesh with and without wraparound is essential to discuss the computation, connectivity, cost, bisection width, and other properties of a molecular mechanical nano-machine. Robert H. Blick et al. (2007) proposed that nano-machines can be improved with the introduction of mechanical computing into the architecture by using terms such as mechanical-resonance and non-linear modification of resonance frequency (Blick et al., 2007). They promise that nanomechanical computing offers a promising new approach to computing, with potential applications in fields like sensing, signal processing, and cryptography, but the scalability of such nano-machines is limited to just the mathematical knowledge of man.

3. Research Methodology

Mechanical nano-computing, or Drexler's Molecular Nano-technology (MNT) is a new and untreaded matter in the field of nano research. The pioneer research is not forty years old yet, but the potential mechanical nano-computers serve is remarkable. Mechanical nano-computers promise to be energy efficient by utilizing mechanical parts and parameters to perform tasks. Moreover, they are presumed to be scalable by detaching and attaching more components or changing the rods. While the earliest rod-sliding model has been deemed unworkable as per the Drexler–Smalley debate (Smalley anticipated a "fat fingers" problem: the apparatus placing the atoms would be too large to fit in the tiny space available), the primitive model still withholds its simplicity and potential, especially in the terms of scalability.

The model, that looks like a network of nodes and connections, is indeed a place for exchange of data and storage of properties, as well as computation through mechanical movements. To analyse them, the proposed 2-

Table 1 Evaluation of static interconnection networks

Network	Diameter	Bisection Width	Arc Connectivity	Cost
Completely connected	1	$\frac{p^2}{4}$	$p-1$	$\frac{p(p-1)}{2}$
Star	2	1	1	$p-1$
Complete Binary Tree	$2\log\left(\frac{p+1}{2}\right)$	1	1	$p-1$
Linear array	$p-1$	1	1	$p-1$
2-D Mesh without Wraparound	$2(\sqrt{p}-1)$	$\sqrt{p}$	4	$2(p-\sqrt{p})$
2-D Mesh with Wraparound	$2\left\lfloor\frac{\sqrt{p}}{2}\right\rfloor$	$2(\sqrt{p})$	4	$2p$
Hypercube	$logp$	$\frac{p}{2}$	$logp$	$\frac{plogp}{2}$
Wraparound K-ary D-cube	$d\left\lfloor\frac{k}{2}\right\rfloor$	$2k^{d-1}$	$2d$	dp

Table 2 Evaluation of static 2-dimensional mesh without wraparound network

Network	**Diameter**	**Bisection Width**	**Arc Connectivity**	**Cost**
2-D Mesh without Wraparound	$2(\sqrt{p}-1)$	$\sqrt{p}$	4	$2(p-\sqrt{p})$

Table 3 Evaluation of static 2-dimensional mesh with wraparound network

Network	**Diameter**	**Bisection Width**	**Arc Connectivity**	**Cost**
2-D Mesh with Wraparound	$2\left\lfloor\frac{\sqrt{p}}{2}\right\rfloor$	$2(\sqrt{p})$	4	$2p$

Dimensional mesh with and without wraparound formulas are to be used in order to:

1) Maximise the arc connectivity: The arc connectivity is a measurement of the minimum number of edges required to disconnect two nodes in a network. Maximising this parameter can enhance the fault tolerance and robustness of the mechanical nano-machine's structure.

2) Minimise the diameter: The diameter of a network of nodes and connections represents the maximum distance between any two nodes in the 2-Dimensional mesh with and without

3) wraparound. A smaller diameter means shorter communication paths and faster data transfer. In a mechanical nano-computer model, the data transfer is required to be quick and efficient, therefore it is necessary to find a point where the diameter of the network is minimised.

4) Maximise the cost: Here, cost refers to the number of edges or connections in the 2-Dimensional mesh with and without wraparound that are related to one another. A higher cost indicates more connections, which can lead to better network performance and reliability. As with arc connectivity, a more interconnected graph can lead to better network performance, and therefore, more robustness in the structure.

5) Minimise the bisection width: The bisection width represents the minimum number of edges that need to be removed to divide the 2-Dimensional mesh with and without wraparound into two disconnected parts. This, by definition, prompts the independence of the connected nano-computers, and their ability to perform freely. A smaller

6) bisection width indicates better connectivity and resilience.

The aim of this research is to calculate results of the different values of the variables M (number of horizontally connected components in a 2-Dimensional mesh with and without wraparound) and N (number of vertically connected components in a 2-Dimensional mesh with and without wraparound). These can also be used to evaluate the parallelisation power of these mechanical nano-computers (as they are theorized to work together, at the same time). Testing the limitations of a mechanical nano-machine's scalable parts is, thus, the final product of this research paper.

4. Paralleisation and Interconnection Network Evaluation of Mechanical Nano-Computers

Evaluating the proposed methodologies is essential to determine the longevity of the proposed nanomechanical models for mechanical computation. We must first consider the structure of a proposed nanomechanical computer.

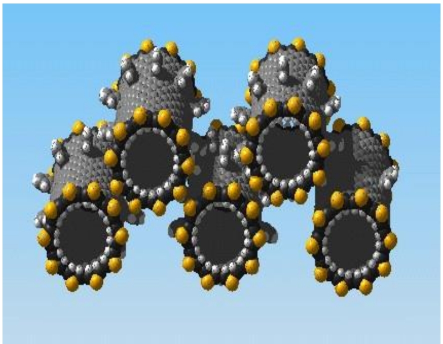


Figure 3 A nano-Pascaline model.

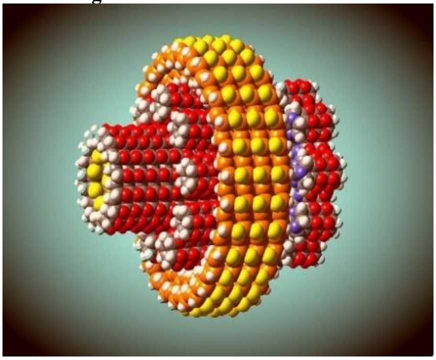


Figure 4 A Nanob.

Assuming a nanomechanical computer (or a mechanical nano-computer) is in the form of a 2-Dimensional mesh when flattened, with or without wraparound, is reasonable for this research. Referring the Encyclopedia of Parallel Computing by David Padua (Padua et al., 2011), we can extract the following table (Table I) for the evaluation of static interconnection networks. Calculations are a necessary segment of this research paper.

We run a python code that calculates the four evaluation factors above to determine the trends in the values for M and N. Ranging these values from 1 to 1000, we compute:

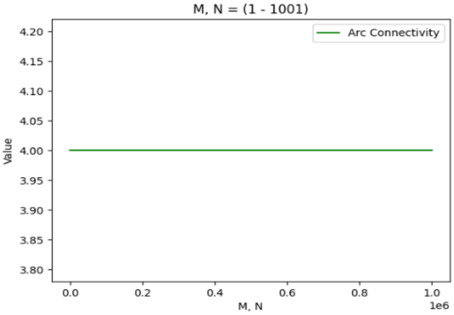
We evaluated the results in terms of graphs and create a table of a few significant results for some values of M and N.

5. Results

After running a code to plot the diameter, bisection width, arc connectivity, and cost of a 2-Dimensional mesh with wraparound shaped mechanical nano-machine model using van Meek et. al research (van Beek et al. 1999).

5.1. Arc Connectivity

We know from the evaluation formula that the arc connectivity of a 2-Dimensional remains constant with or without wraparound. Therefore, the graphs for the arc connectivity remain constant and uniform at $y = 4 \ \forall \ x \in \{1 - 1000\}$ (here $x = M, N$). The graphs for the arc connectivity of 2-Dimensional mesh with and without wraparound are given below.



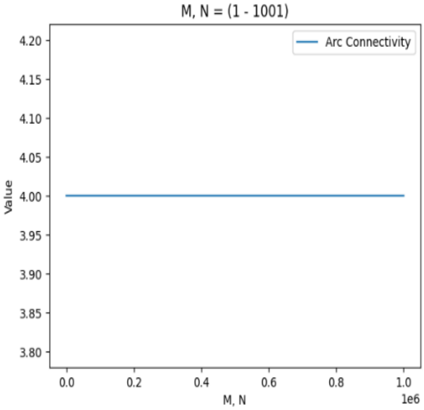
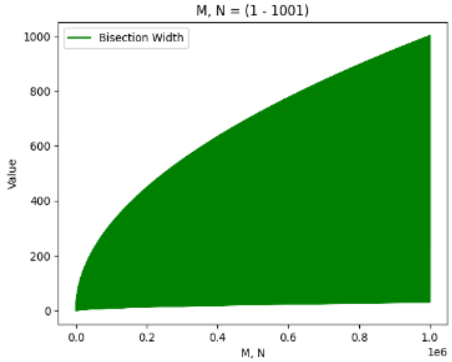


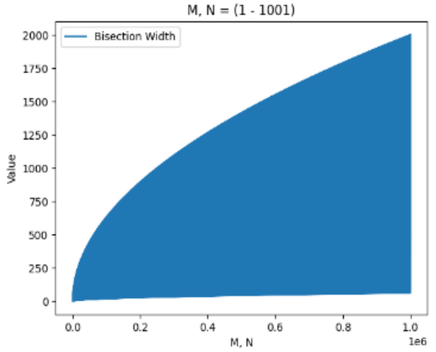
Figure 5 The graph for the arc connectivity of a 2-Dimensional mesh with no wraparound & The graph for the arc connectivity of a 2-Dimensional mesh with wraparound.

This shows that regardless of the number of nanogears or nodes in the mechanical nano-computer, the minimum number of edges required to disconnect two nodes (or nanogears) in a model is 4.

On the other hand, the bisection width of the two increase sharply until around 0.2 * 1e6 nanogears (Fig. 7.), after which they begin to flatten out. A similar trend is observed with the diameter of the nano-computer (Fig. 8.). From this we can find out that the best values of both of the components is before the graph starts flattening. This implies that the ideal values of M and N are around 448.

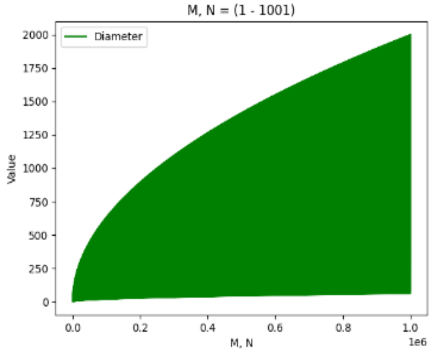


(a)

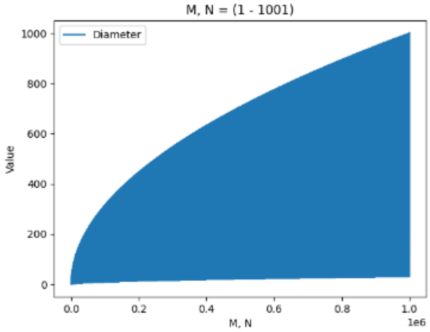


(b)

Figure 6 The graph for the bisection widths of a (a) 2-Dimensional mesh without wraparound and (b) 2-Dimensional mesh with wraparound for the values of M and N ∈ {1 – 1000}.



(a)



(b)

Figure 7 The graph for the diameters of a (a) 2-Dimensional mesh without wraparound and (b) 2-Dimensional mesh with wraparound for the values of M and N ∈ {1 – 1000}.

Finally, the cost of both 2-Dimensional wraparound and no wraparound mesh create a steep, straight slope that show increase in cost as M x N increase in value, reaching a maximum of approximately 2000 in both the cases. We can visualise this better if we fix the value of N = 2, imaging this to be a 2-Dimensional mesh with no intermediary nodes, just a rectangular border.

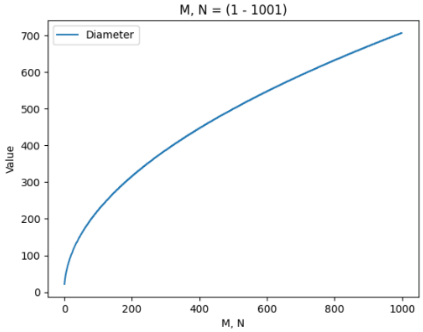


Figure 8 The graph for the diameters of a 2-Dimensional mesh (with and without wraparound for M ranging from 1 to 1000, and N = 2.

Keeping all of these in mind, we can conclude that the number of nanogears (nodes) in a single mechanical nano-computer can ideally be around 448, as we are required to minimise both the diameter and the bisection width. Having more than 400 nanogears to store and encode data in a singular mechanical nano-machine is remarkable. It nods at the scalability power of the MNT and mechanical nano-machine.

6. Conclusion (Future Directions)

The scalability of mechanical nano-computers based on the Drexler MNT model of a mechanical nano-machine with nanogears (nodes) and rods (connections) can be scaled up to 448 individual nanogears. These nanogears provide a platform to encode information and act as a 'memory' for the nano-machine. Further, these nanogears alight with the nano-gears of other nano-machine components to perform the mechanical calculations, in a Pascaline method.

The mechanical calculations of a nano-computer are theorized to be far more efficient in terms of energy consumption as compared to the electronic nano-computer. The scalability of mechanical nano-computers is also hypothesized to be remarkable. These achievements make the mechanical nano-machine especially useful in the field of medicine. Nanomedicine and nano delivery systems (for drug transmissions and transfer) are a new but rapidly developing science. These consist of the carriage of nanoscale materials through a body's blood stream and fluids, often the drugs that are to participate in drug-drug transmissions. Nanotechnology offers multiple benefits in treating chronic human diseases by site-specific, and target-oriented delivery of precise medicines in precise locations. Replacing the electronic components of these nano-tech devices with nanogears (with encoded information about the drug and the location of the organ affected) of a nano-mechanical device can help tremendously. The scalability of a mechanical nano-machine further assists in storing more information about the drug delivery system, and creating faster transfer of drugs to the specified target.

Mechanical nano-computers can potentially be improved with automation systems, distribution of data amongst nanogears or nodes, and assist in nano-robotics. Cochlear implants can be automated through specially designed mechanical nano-robots for surgical environments. The ability to re-join damaged nerves to improve optical conditions at a molecular level will be streamlined with the introduction of like-sized nano-robots that are both scalable and efficient.

The applications of mechanical nano-machines, especially as mechanical nano-robots. For future work, we would like to limit the environmental conditions of these hypothetical mechanical nano-machines to bio-atmospheres, such as the human body, and mathematically observe their behaviours. We hope to contribute to the rapidly growing research in the modelling of mechanical nano-machines, especially in medical fields.

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