Embedding Techniques in Interconnection Networks and Cheminformatics

SYNOPSIS

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SYNOPSIS

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1 Introduction

The field of mathematics plays a vital role in various fields. One of the important areas in mathematics is Graph Theory which is used in structural models. This structural arrangement of various objects or technologies lead to new inventions and modifications in the existing environment for enhancement in those fields. Created in the works of Leonhard Euler (1707-1783) in the eighteenth century and developed by Arthur Cayley (1821-1895) and James. J. Sylvester (1814-1897) in the nineteenth century, Graph Theory became in the twentieth century an essential tool in many areas of science and technology. Graph theoretical ideas are highly utilized by computer science applications, especially in research areas of computer science such as data mining, image segmentation, clustering, image capturing, networking and so on. For example, a data structure can be designed in the form of tree which in turn utilizes vertices and edges. Thus graph theory is used to model the relationship between a network of vertices and edges.

One of the most important problems facing technology today is the development of scientific supercomputers. Computer science experts believe that future supercomputers will be based on large-scale parallel processing. Such a computer will have a system consisting of many processors and memories. An essential component of such computers is the interconnection network providing communication among the processors and memories of the system. The advent of very large scale integration (VLSI) makes it possible to put more processors which are faster and have more memory on a single chip. Thus, the interconnection networks of future multiprocessor computing systems may be very complex. Indeed, we are seeing this trend today. The Connection Machine developed by Thinking Machines Inc. consists of 216 single-bit processors all working in parallel!

Interconnection networks are often modeled by graphs. The vertices of the graph correspond to processing elements, memory modules, or just switches. The edges correspond to communication lines. If communication is one-way, the graph is directed; otherwise, the graph is undirected. Here is an incomplete list of graph properties that a good model might possess: simple and efficient routing algorithms, small diameter, high connectivity and small degree. Also, one would wish the interconnection network to be as efficient as possible. Ideally one wants each processor to send a message and each memory module to receive a message with each ”clock tick.” One approach to this problem is to design networks with lots of switching nodes connected in such a way as to ensure multiple memory-processor paths. There is also the ”lay-out problem”, (i.e), the problem of embedding the graph in a 2 or 3 dimensional Euclidean space in a manner that can be realized in hardware. Additionally, it is desirable that the longest wire link be as short as possible since timing problems arise otherwise. Finding graphs that satisfy these conditions can be a formidable task; in fact, the properties of high connectivity and small degree seem to be inversely proportional to each other. Consequently, in a particular application, trade-offs must be made. Vertex symmetric graphs are especially well suited as models for interconnection networks because these graphs have the property that the graph viewed from any vertex looks the same. Moreover, the symmetry of the graph minimizes congestion, as traffic is distributed uniformly over all vertices.

2 Preliminaries

2.1 Graph Embedding

An interconnection network of a system provides logically a specific way in which all components of the system are connected. In this, the simulation of one architecture by another is important. The problem of simulating one network by another is modeled as a *graph embedding problem*. The need for efficient embedding stems from atleast two different directions. If a network A can be embedded in a network B, then all the algorithms developed for parallel processing with network A can be easily transported onto another processor network B. Secondly, mapping parallel algorithms onto parallel architectures often leads to embedding of the control or data flow graphs of the algorithms into the underlying graph of the network. While the general problem of graph embedding is difficult, by exploiting the special structure of the interconnection schemes, a number of results relating to optimal embedding of one class of networks into another have been developed. Embedding the structures may result in substantial savings in communication time. The transmission delay is an important measure for the global communication efficiency of an interconnection network.

There are several results on the embedding problem of various architectures such as 1-vertex-fault-tolerant cycles embedding on folded hypercubes [37], trees on cycles [9], trees on stars [38], hypercubes into grids [5], complete binary tree into grids [30], grids into grids [34], ladders and caterpillars into hypercubes [7], binary trees into hypercubes [11], complete trees into hypercubes [4], incomplete hypercube in books [12], m-sequencial k-ary trees into hypercubes [33], ternary tree into hypercube [14], enhanced and augmented hypercube into complete binary tree [25], circulant into arbitrary trees, cycles, certain multicyclic graphs and ladders [17], hypercubes into cylinders, snakes and caterpillars [26] and path embedding on folded hypercubes [35].

The formal definition of an embedding is as follows:

Definition 2.1 [5] *Let G and H be finite graphs with n vertices. An embedding f of a guest graph G into a host graph H is defined as follows:*

(i) f *is a bijective map from* $V(G) \rightarrow V(H)$

(ii) P_f *is an one-to-one map from* $E(G) \rightarrow \{P_f(u,v) : P_f(u,v)$ *is a path in* H *between* $f(u)$ *and* $f(v)$ *for* $(u,v) \in E(G)\}$.

The graph G that is being embedded is called a *virtual graph* or a *guest graph* and H is called a *host graph*. Some authors use the name $labelling$ instead of embedding [4].

Dilation, expansion, congestion and wirelength are some cost criteria which determine the quality of an embedding.

Definition 2.2 *If* $e = (u, v) \in E(G)$*, then the length of* $P_f(u, v)$ *in* H *is called the dilation of the edge* e*. The maximum dilation over all edges of* G *is called the dilation of the embedding* f*.*

Definition 2.3 *The expansion of an embedding* f *is the ratio of the number of vertices of* H *to the number of vertices of* G*.*

Definition 2.4 *The edge congestion of an embedding* f *of* G *into* H *is the maximum number of edges of the graph* G *that are embedded on any single edge of* H*.*

In other words,

$$EC_f(G, H) = \max EC_f(G, H(e)),$$

where the maximum is taken over all the edges e *of* H *and the minimum edge congestion of* G *into* H *is defined as*

$$EC(G, H) = \min EC_f(G, H)$$

where the minimum is taken over all embeddings f *of* G *into* H*.*

The edge congestion problem of a graph G is to find an embedding of G into H that induces $EC(G, H)$.

Definition 2.5 *The wirelength of an embedding* f *of* G *into* H *is given by*

$$WL_f(G, H) = \sum_{(u,v)\in E(G)} d_H(f(u), f(v)) = \sum_{e\in E(H)} EC_f(G, H(e))$$

where $d_H(f(u), f(v))$ *denotes the length of the path* $P_f(u, v)$ *in* H*.*

Definition 2.6 *The wirelength of embedding G into H is defined as*

$$WL(G,H) = \min WL_f(G,H)$$

where the minimum is taken over all embeddings f of G into H.

The edge isoperimetric problem [15] is used to solve the wirelength problem when the host graph is a path and is NP-complete [13]. The following two versions of the edge isoperimetric problem of a graph $G(V,E)$ have been considered in the literature [6].

Problem 1 : Find a subset of vertices of a given graph, such that the edge cut separating this subset from its complement has minimal size among all subsets of the same cardinality. Mathematically, for a given m, if $\theta_G(m) = \min_{A\subseteq V,\, |A|=m} |\theta_G(A)|$ where $\theta_G(A) = \{(u,v) \in E : u \in A, v \notin A\}$, then the problem is to find $A \subseteq V$ and $|A| = m$ such that $\theta_G(m) = |\theta_G(A)|$.

Problem 2 : Find a subset of vertices of a given graph, such that the number of edges in the subgraph induced by this subset is maximal among all induced subgraphs with the same number of vertices. Mathematically, for a given m, if $I_G(m) = \max_{A\subseteq V,\, |A|=m} |I_G(A)|$ where $I_G(A) = \{(u,v) \in E : u,v \in A\}$, then the problem is to find $A \subseteq V$ and $|A| = m$ such that $I_G(m) = |I_G(A)|$.

For a given m, where $m = 1, 2, \ldots, |V|$, we consider the problem of finding a subset A of vertices of G such that $|A| = m$ and $|\theta_G(A)| = \theta_G(m)$. Such subsets are called optimal with respect to Problem 1. We say that optimal subsets are nested if there exists a total order $\mathcal{O}$ on the set V such that for any $m = 1, 2, \ldots, n$, the collection of the first m vertices in this order is an optimal subset. In this case we call the order $\mathcal{O}$ an optimal order [15, 6]. This implies that $WL(G, P_{|V|}) = \sum_{m=1}^{|V|} \theta_G(m)$, where P_n is a path on n vertices. Again, a subset A of vertices of G such that $|A| = m$ and $I_G(m) = |I_G(A)|$ is said to be optimal with respect to Problem 2.

If a subset of vertices is optimal with respect to Problem 1, then its complement is also an optimal set. However, it is not true for Problem 2 in general, although this is indeed the case if the graph is regular [6]. In the literature, Problem 2 is defined as the *maximum subgraph problem* [13]. For a regular graph, Problem 1 and Problem 2 are equivalent.

2.2 Topological Indices

Indices are more complex methods to represent the structural properties of a graph since they involve the comparison of a measure over another. A high index shows a developed network and is also an indicator of the shape of a network. Thus, a topological index is a real number related to a chemical graph. A chemical graph is a graph in which every vertex has a degree = 4. Each molecule is described by a chemical graph. The vertices of this graph denote the atoms and the edges are the bonds of the molecule. Indices have applications in Nanotechnology, in Drug design to develop Quantitative Structure Toxicity Relationship (QSTR), Quantitative Structure Property Relationship (QSPR), Quantitative Structure Activity Relationship (QSAR) and Phenylenic nanotubes and nanotori. Padmakar V. Khadikar introduced a new topological index called *Padmakar - Ivan index* [20, 22], which is abbreviated as PI index. In a series of papers, Khadikar et. al. computed the PI index of some chemical graphs [22, 21, 23]. Ali Reza Ashrafi and Amir Loghman computed the PI index of a zig- zag polyhex nanotube [2] and they also computed PI index of some benzenoid graphs [2].

Definition 2.7 [20] *The PI index of a graph G is defined as $PI(G) = \sum[\eta_{eu}(e|G) + \eta_{ev}(e|G)]$, where for the edge $e = (u, v), \eta_{eu}(e|G)$ is the number of edges of G lying closer to u than $v; \eta_{ev}(e|G)$ is the number of edges of G lying closer to v than u and summation goes over all edges of G. When there is no ambiguity, we denote $PI(G)$ by PI and define $PI = \sum_{e \in E}[\eta_{eu} + \eta_{ev}]$.*

In this thesis, we use embedding as a tool to compute PI index of graphs.

3 Outline of the Thesis

This thesis pertains to the study of embedding one interconnection network into another and use embedding concepts to obtain PI index of certain chemical graphs. The thesis contains seven chapters.

In Chapter 1, we present a few basic graph-theoretic concepts and their applications, and an overview of the thesis.

In Chapter 2, we record a brief history of the embedding concepts and a concise survey of work done on embedding problems.

In Chapter 3, we determine the exact wirelength of folded hypercubes into cylinders and torii.

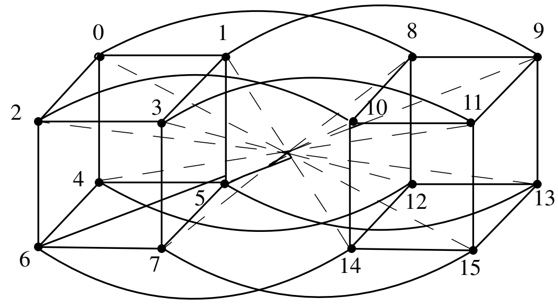

Figure 1: Folded hypercube FQ^4 with dashed lines representing the complementary edges

One of the most popular variants of the hypercube is the folded hypercube, which can be constructed by adding a link to every pair of nodes with complementary address. The folded hypercube has been shown to be able to improve the system's performance over a regular hypercube in many measurements [1, 39].

The folded hypercube is represented by FQ^r and is defined as follows:

Definition 3.1 [32] *For two vertices $x = x_1x_2 \cdots x_r$ and $y = y_1y_2 \cdots y_r$ of Q^r, (x, y) is a complementary edge if and only if the bits of x and y are complements of each other, that is, $y_i = \overline{x_i}$ for each $i = 1, 2, ..., r$. The r-dimensional folded hypercube, denoted by FQ^r is an undirected graph obtained from Q^r by adding all complementary edges. See Figure 1.*

It is easy to see that any r-dimensional folded hypercube FQ^r can be viewed as $G(0Q^{r-1}, 1Q^{r-1}; C + \overline{C})$ where $0Q^{r-1}$ and $1Q^{r-1}$ are two $(r-1)$-dimensional hypercubes with the prefix 0 and 1 of each vertex respectively, and $C = \{(0u, 1u) : 0u \in V(0Q^{r-1})$ and $1u \in V(1Q^{r-1})\}, \overline{C} = \{(0u, 1\overline{u}) : 0u \in V(0Q^{r-1})$ and $1\overline{u} \in V(1Q^{r-1})\}$

[41].

Definition 3.2 [26] *The* 2*-dimensional grid is defined as* $P_{d_1} \times P_{d_2}$ *, where* $d_i \geq 2$ *is an integer for each* i *= 1, 2. The cylinder* $C_{d_1} \times P_{d_2}$*, where* $d_1, d_2 \geq 3$ *is a* $P_{d_1} \times P_{d_2}$ *grid with a wraparound edge in each row. See Figure 2(a).*

It is clear that the vertex set of $P_{d_1} \times P_{d_2}$ is $V = \{x_1x_2 : 0 \leq x_i \leq d_i - 1, i = 1, 2\}$ and two vertices $x = x_1x_2$ and $y = y_1y_2$ are linked by an edge, if $|x_1 - y_1| + |x_2 - y_2| = 1$.

Lemma 3.3 For $i = 1, 2, \cdots, 2^{\lfloor r/2 \rfloor} - 1$,

$$R_i^{lex} = \begin{pmatrix} 0, & 1 \times 2^{\lfloor r/2 \rfloor}, & \cdots, & (2^{\lceil r/2 \rceil} - 1) \times 2^{\lfloor r/2 \rfloor} \\ 1, & 1 \times 2^{\lfloor r/2 \rfloor} + 1, & \cdots, & (2^{\lceil r/2 \rceil} - 1) \times 2^{\lfloor r/2 \rfloor} + 1 \\ \cdots, & \cdots, & \cdots, & \cdots \\ i-1, & 1 \times 2^{\lfloor r/2 \rfloor} + i - 1, & \cdots, & (2^{\lceil r/2 \rceil} - 1) \times 2^{\lfloor r/2 \rfloor} + i - 1 \end{pmatrix}$$

is a composite set in FQ^r.

$Notation$: Let $C_0, C_1, \cdots, C_{2^{\lceil \frac{r}{2} \rceil} - 1}$ denote the columns of L. Let $[C_i, C_{i+1}, \cdots, C_j]$ denote the submatrix of L constituted by the columns $C_i, C_{i+1}, \cdots, C_j$. Let $\overline{C}_j = \{l_{nj}, l_{(n-1)j}, \cdots, l_{1j}\}$

Lemma 3.4 For $j = 1, 2, \cdots, 2^{\lceil r/2 \rceil - 1}$,

$$\mathtt{C}_j^{lex} = [C_j, C_{j+1}, \cdots, C_{2^{\lfloor r/2 \rfloor} - 1}, C_{1 + (2^{\lfloor r/2 \rfloor} - 1)}, \cdots, C_{j + (2^{\lceil r/2 \rceil - 1} - 1)}]$$

is a composite set in FQ^r.

Lexicographic embedding. The lexicographic embedding [5] of FQ^r with lexicographic labeling 0 to $2^r - 1$ into $C_{\lfloor \frac{r}{2} \rfloor} \times P_{\lceil \frac{r}{2} \rceil}$ is an assignment of a label to the vertex $x_1 x_2$ of $C_{\lfloor \frac{r}{2} \rfloor} \times P_{\lceil \frac{r}{2} \rceil}$ as

$x_1 + 2^{\lfloor \frac{r}{2} \rfloor} x_2$,if $0 \leq x_2 \leq 2^{\lceil \frac{r}{2} \rceil - 1} - 1$,

$x_1 + 2^{\lfloor \frac{r}{2} \rfloor}(3.2^{\lceil \frac{r}{2} \rceil - 1})$, if $2^{\lceil \frac{r}{2} \rceil - 1} \leq x_2 \leq 2^{\lceil \frac{r}{2} \rceil} - 1 : x_2$ even

$x_1 + 2^{\lfloor \frac{r}{2} \rfloor}(3.2^{\lceil \frac{r}{2} \rceil - 1} - x_2)$, if $2^{\lceil \frac{r}{2} \rceil - 1} \leq x_2 \leq 2^{\lceil \frac{r}{2} \rceil} - 1 : x_2$ odd

where $0 \leq x_1 \leq 2^{\lceil \frac{r}{2} \rceil} - 1$. This lexicographic embedding is denoted by *lex*.

Theorem 3.5 *The lexicographic embedding lex of the folded hypercube FQ^r into the cylinder $C_{2^{\lfloor r/2 \rfloor}} \times P_{2^{\lceil r/2 \rceil}}$ induces a minimum wirelength $WL(FQ^r, C_{2^{\lfloor r/2 \rfloor}} \times P_{2^{\lceil r/2 \rceil}})$.*

Theorem 3.6 *The exact wirelength of embedding FQ^r into the cylinder $C_{2^{\lfloor r/2 \rfloor}} \times P_{2^{\lceil r/2 \rceil}}$ is given by,*

$$\begin{aligned} WL(FQ^r, C_{2^{\lfloor r/2 \rfloor}} \times P_{2^{\lceil r/2 \rceil}}) \\ &= \sum_{i=1}^{2^{\lfloor r/2 \rfloor} - 1} i((r+1)2^{\lceil r/2 \rceil}) - 2|E(FQ^r(L_{i2^{\lfloor r/2 \rfloor}})| + (r+1)2^{r-1} \\ &\quad +2(r-1)2^{r-2} \\ &= \sum_{i=1}^{2^{\lfloor r/2 \rfloor} - 1} i((r+1)2^{\lceil r/2 \rceil}) - 2|E(FQ^r(L_{i2^{\lfloor r/2 \rfloor}})| + r2^r \end{aligned}$$

The above results have been presented at the 4^{th} Workshop on UNESCO-HP ”Brain Gain Initiative” in conjunction with 3^{rd} Kuwait Conference on e-Services and e-Systems (KCESS 2012), Kuwait, in December 18-20, 2012. Also, these results have been *submitted* for publication to **Information Processing Letters**.

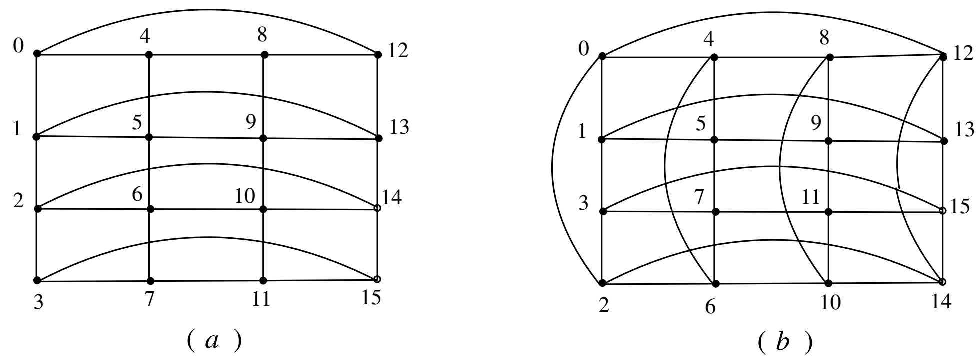

Figure 2: (*a*) Cylinder $C_4 \times P_4$ (*b*) Torus $C_4 \times C_4$

The family of torii is one of the most popular interconnection networks due to its desirable properties such as regular structure, ease of implementation and good scalability. In recent years, the theory of torus embedding has found many applications. It has been used in many practical systems such as Cray T3D, Cray T3E, Fujitsu AP3000, Ametak 2010, Intel Touchstone and so on [28].

Definition 3.7 [24] *An n-dimensional torus $C(m_1, m_2, ..., m_n)$ is defined as the Cartesian product of n cycles $C_{m_1} \times C_{m_2} \times ... \times C_{m_n}$, where C_{m_i} is the cycle graph with m_i vertices. See Figure 2(b).*

Lemma 3.8 $R_1^{lex} = \{0, 1\times 4, 2\times 4, \cdots, (2^{r-2}-1)\times 4, 1, 1\times 4+1, 2\times 4+1, \cdots, (2^{r-2}-1)\times 4+1\}$ *is a composite set in FQ^r.*

Lemma 3.9 $R_2^{lex} = \{0, 1\times 4, 2\times 4, \cdots, (2^{r-2}-1)\times 4, 2, 1\times 4+2, 2\times 4+2, \cdots, (2^{r-2}-1)\times 4+2\}$ *is a composite set in FQ^r.*

Lemma 3.10 *Let $A = 0, 1, \cdot\cdot\cdot, 2^{r-1}-1$. For $j = 1, 2, \cdot\cdot\cdot, 2^{r-3}-1$, let $B_j = A \backslash \{0, 1, \cdot\cdot\cdot, 4j-1\} \cup \{2^r-1, 2^r-2, \cdot\cdot\cdot, 2^r-4j\}$, for j even and for j odd, let*

$B_j = A\backslash\{0,1,\cdots,4j-1\}\cup B_{j-1}\cup\{2^r-(4j+1),2^r-(4j+2),2^r-(4j+3),2^r-(4j+4)\}$ *is a composite set in* FQ^r.

Theorem 3.11 *The lexicographic embedding lex of the folded hypercube* FQ^r *into the torus* $C_4 \times C_{2^{r-2}}$ *induces a minimum wirelength* $WL(FQ^r, C_4 \times C_{2^{r-2}})$.

Theorem 3.12 *The exact wirelength of embedding* FQ^r *into the cylinder* $C_4 \times C_{2^{r-2}}$ *is given by,*

$$\begin{aligned} & WL(FQ^r, C_4 \times C_{2^{r-2}}) \\ &\qquad = EC(R_i) + EC(C_j) \\ &\qquad = 2^{2r-3} - 2^{r-1} + \sum_{j=1}^{2^{r-3}} (j(r+1)2^{r-1}) - 2|E(FQ^r(L_{j2^{r-1}}))| \end{aligned}$$

The above results have been *submitted* for publication to **Journal of Interconnection Networks**.

In Chapter 4, we determine the exact wirelength of circulant networks into a family of grids.

The circulant network is a natural generalization of double loop network and have been used for decades in the design of computer and telecommunication networks due to their optimal fault-tolerance and routing capabilities [8]. It is also used in VLSI design and distributed computation.

From a theoretical point of view, there are thousands of publications analyzing their algebraic properties. From a more practical perspective, circulant graphs have been employed in several applications. In the sixties, these graphs were used to

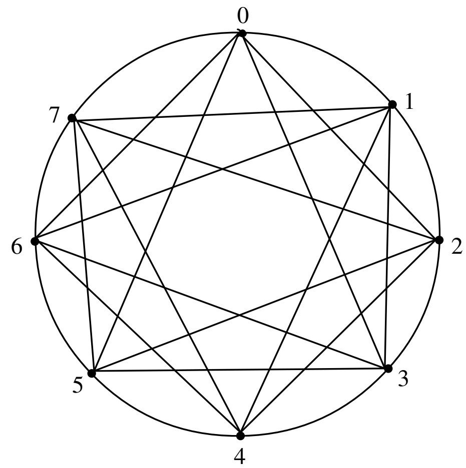

Figure 3: Circulant graph $G(8; \{1, 2, 3\})$

build interconnection networks for distributed and parallel systems. In the seventies, circulant graphs constituted the basis for designing certain data alignment networks for complex memory systems. In the eighties, several optimizations related to the diameter minimization of degree four circulant graphs, enhanced the applicability to the design of efficient interconnection networks. Nowadays, the analysis and characterization of circulant graphs and their applications still constitute active research areas. In addition, these graphs are regular, vertex-symmetric, maximally connected and, after an adequate transformation, they can be represented as mesh-connected topologies [3].

Definition 3.13 [17] *A circulant undirected graph, denoted by* $G(n; \pm S)$ *where* $S \subseteq \{1, 2, \cdot\cdot\cdot, \lfloor n/2 \rfloor\}, n \geq 3$ *is defined as a graph consisting of the vertex set* $V = \{0, 1, \cdot\cdot\cdot, n-1\}$ *and the edge set* $E = \{(i, j) : |j - i| \equiv s(mod n), s \in S\}$*. See Figure 3.*

Proposition 3.0.1 [17] *The number of edges in a maximum subgraph on* k *vertices of*

$G(n;\pm S), S=\{1,2,\cdots,j\}, 1\leq j\leq \lfloor n/2\rfloor, n\geq 3$ *is given by,*

$$\xi \;=\; \begin{cases} k(k-1)/2, & k\leq j+1 \\ kj-j(j+1)/2, & j+1<k\leq n-j \\ (1/2)\{(n-k)^2+(4j+1)k-(2j+1)n\}, & n-j<k\leq n \end{cases}$$

Proposition 3.0.2 [17] *A set of k consecutive vertices of $G(n;\pm 1), 1\leq k\leq n$ induces a maximum subgraph of $G(n;\pm S)$ where $S=\{1,2,\cdots,j\}, 1\leq j\leq \lfloor n/2\rfloor, n\geq 3$.*

Theorem 3.14 *The maximum subgraph on the set of all k vertices of $G(n;\{1,2,\cdots,j\})$, for $k<j$, is a complete graph on k vertices.*

An $l\times m$ grid with l rows and m columns is represented by $M[l\times m]$.

Lemma 3.15 *For m odd,*

$$R_1 \;=\; \left\{\; 0,\;\; 1\times 4,\;\; \cdots,\;\; (m-1)\times 4 \;\right\}$$

$$R_2 \;=\; \left\{\; 1,\;\; 1\times 4+1,\;\; \cdots,\;\; (m-1)\times 4+1 \;\right\}$$

and for m even, we get,

$$R_1 \;=\; \left\{ \begin{array}{cccc} 0, & 1\times 4, & \cdots, & \lceil n/2\rceil-4, \\ & \lceil n/2\rceil+3, & (\lceil n/2\rceil+3)+(4\times 1), & \cdots, \\ & (\lceil n/2\rceil+3)+(4\times((m/2)-1)) & & \end{array} \right\}$$

$$R_2 \;=\; \left\{ \begin{array}{cccc} 1, & 1\times 4+1, & \cdots, & (\lceil n/2\rceil-4)+1, \\ & (\lceil n/2\rceil+3)-1, & ((\lceil n/2\rceil+3)+(4\times 1))-1, & \\ & \cdots, & (\lceil n/2\rceil+3)+(4\times(m/2-1))-1 & \end{array} \right\}$$

and R_3 which is isomorphic to R_1 in both cases are maximum subgraphs in $G(n;\{1,2,\cdots,\lfloor n/2\rfloor-1\})$.

Lemma 3.16 *For* $1 \leq j \leq m-1$, $C_j = \{0, 1, 2, \cdots, 4j-1\}$, *is maximum in* $G(n; \{1, 2, \cdots, \lfloor n/2 \rfloor - 1\})$.

Theorem 3.17 *The embedding* f *of the circulant network* $G(n; \{1, 2, \cdots, \lfloor n/2 \rfloor - 1\})$ *into the grid* $M[4 \times m]$*, where* $m > 2$ *induces a minimum wirelength* $WL(G(n; \{1, 2, \cdots, \lfloor n/2 \rfloor - 1\}), M[4 \times m])$.

Theorem 3.18 *The exact wirelength of embedding* $G(4n; \{1, 2, \cdots, \lfloor (2n-1) \})$ *into the grid* $M[4 \times n]$*, where* $n \geq 2$ *is given by,*

$$\begin{aligned} WL(G(4n; \{1, 2, \cdots, (2n-1)\})), M[4 \times n]) &= 2(5n^2 + 6n - 10) + \\ &\sum_{j=2}^{n-1} [8j(2n-1) - 16(n-j)^2 - 4j(8n-3) + 4n(4n-1)] \end{aligned}$$

The contents of this chapter have been *published* in the **International Journal of Pure and Applied Mathematics**, Vol. 86, no. 6, 883–891, 2013.

In Chapter 5, we determine the exact wirelength of hypercubes into extended banana trees and arbitrarily fixed generalized banana trees.

The hypercube is a very popular interconnection network for parallel computation since it possesses many attractive properties such as low diameter, relatively small degree, recursive structure and so on. One of the biggest reasons for the popularity of the hypercube is its ability to efficiently embed many parallel architectures [5, 7, 11].

Definition 3.19 [40] *For* $r \geq 1$*, let* Q^r *denote the graph of* r*-dimensional hypercube. The vertex set of* Q^r *is formed by the collection of all* r*-dimensional binary*

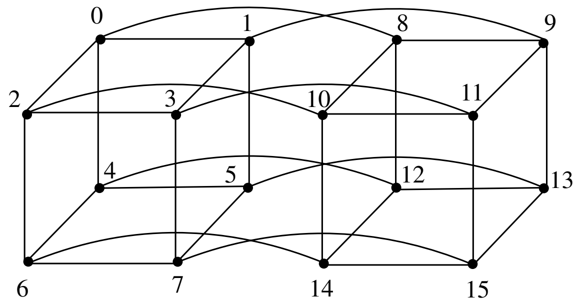

Figure 4: Hypercube Q_4

representations. Two vertices $x, y \in V(Q^r)$ *are adjacent if and only if the corresponding binary representations differ exactly in one bit. See Figure 4.*

Equivalently if $n = 2^r$, then the vertices of Q^r can also be identified with integers $0, 1, ..., n-1$ so that if a pair of vertices i and j are adjacent then $i - j = 2^p$, for some $p \geq 0$.

Definition 3.20 [27] *An incomplete hypercube on* i *vertices of* Q^r *is the subcube induced by* $\{0, 1, \cdots, i-1\}$ *and is denoted by* L_i, $1 \leq i \leq 2^r$.

Definition 3.21 [10] *A Banana Tree* $B(n, k)$*, is a graph obtained by connecting one leaf of each of* n *copies of a* k*-star graph with a single root vertex that is distinct from all the stars.*

Definition 3.22 *An Extended Banana Tree denoted by* $B(n_1, n_2, \cdots, n_m; k_1, k_2, \cdots, k_m)$ *is a graph obtained by connecting one leaf of each of* $\{n_1, n_2, \cdots, n_m\}$ *copies of* $\{k_1, k_2, \cdots, k_m\}$ *- star graphs with a single root vertex that is distinct from all the stars. See Figure 5(a).*

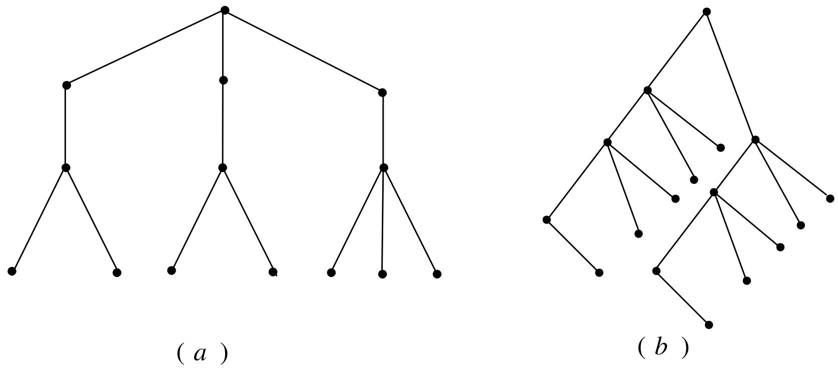

Figure 5: (a) $B(2,1;4,5)$ (b) $T(2,3,5)$

Theorem 3.23 *The exact wirelength of embedding Q^r into $B(n_1, n_2, \cdots, n_m; k_1, k_2, \cdots, k_m)$, is given by*

$$WL(Q^r, B(n_1, n_2, \cdots, n_m; k_1, k_2, \cdots, k_m)) = r[2^r - 2(n_1 + n_2 + \cdots + n_m) - 1] + r[\sum_{i=1}^{m} k_i - m] - 2[\sum_{i=1}^{m} r_i 2^{r_i - 1} - r_i] - (r_m - 1) + r[\sum_{i=1}^{m} k_i] - 2[\sum_{i=1}^{m} r_i 2^{r_i - 1}] - r_m$$

Definition 3.24 [19] *Consider a set of caterpillars, having equal (or fixed) diameter, in which one of the penultimate vertices is of arbitrary degree and all other internal vertices including the other penultimate vertex is of fixed even degree. Merge an end-vertex adjacent to the penultimate vertex of fixed even degree of each such caterpillars together. The rooted tree thus obtained is called Arbitrarily Fixed Generalized Banana Tree. See Figure 5(b).*

For our discussion, we describe the Arbitrarily Fixed Generalized Banana Tree as follows: Let $T(l, n, k)$ be the rooted Arbitrarily Fixed Generalized Banana Tree having l copies of $C(n, k)$ where $C(n, k)$ denotes a caterpillar. A caterpillar is a tree such that removing the vertices of degree - 1 called the *legs* yields a path, called the *spine*. Here n

represents the number of vertices of the spine and k represents the number of vertices of the legs. We also impose the condition that $l(2^i) = 2^r + 1$.

Theorem 3.25 *The exact wirelength of embedding Q^r into $T(l,n,k)$ is given by,*
$WL(Q^r, T(l,n,k))) = r[2^r - 2(n_1 + n_2 + \cdots + n_m) - 1] + r[\sum_{i=1}^{m} k_i - m] - 2[\sum_{i=1}^{m} r_i 2^{r_i - 1} - r_i]$

The results obtained in this chapter have been *presented* in the **International Conference on Mathematics in Engineering and Business Management (ICMEB 2012),** Chennai, India and *accepted* for publication in the **Journal of Combinatorial Mathematics and Combinatorial Computing**.

In Chapter 6, we determine the exact wirelength of Petersen graphs into certain trees.

In 1950 a class of generalized Petersen graphs was introduced by Coxeter and around 1970 was popularized by Frucht, Graver and Watkins. The Petersen graph is certainly one of the most famous objects that graph theorists have come across. This graph is a counterexample to many conjectures: for example, it is not 1-factorizable despite being cubic and without bridges (Taits conjecture), and it is not hamiltonian. But being 3-transitive (that is, its automorphism group is transitive on directed paths of length 3), it is highly symmetric; however, it is not a Cayley graph! Many additional facts about the Petersen graph can be found in [29]. The Petersen graph appeared in the chemical literature as the graph that depicts a rearrangement of trigonal bipyramid complexes $XY5$ with five different ligands when axial ligands become equatorial and equatorial ligands become axial [31].

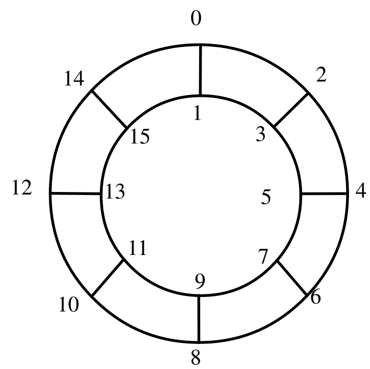

Figure 6: Circular ladder $P(8, 1)$

Definition 3.26 [40] *The generalized Petersen graph* $P(m, n), 1 \leq m \leq n-1$ *and* $n \neq 2m$*, consists of an outer* n*-cycle* $u_1, u_2, \cdots, u_n$*, a set of* n *spokes* $(u_i, v_i), 1 \leq i \leq n$*, and* n *inner edges* (v_i, v_{i+m}) *with indices taken modulo* n*. It is a 3-regular graph and contains* $2n$ *vertices and* $3n$ *edges. See Figure 6.*

Parallel labeling [16]. For $1 \leq i \leq n$, we call the vertices u_i and v_i of $P(m, n)$ as outer rim and inner rim vertices respectively and label the vertices u_i and v_i as $2i-2$ and $2i-1$ respectively. We call this labeling as *parallel labeling* of the generalized Petersen graph $P(m, n)$.

We know that the generalized Petersen graph $P(n, 1), n \geq 3$ is the circular ladder $K_2 \times C_n$.

Proposition 3.0.3 [16] *The number of edges in a subgraph induced by any set of* k *vertices of* $P(n, 1), 3 \leq k \leq n$ *is atmost* $k + \lfloor k/2 \rfloor - 2$ *for* $n > 3$ *.*

Proposition 3.0.4 [16] *Let* H *be a subgraph of* $P(n, 1)$ *induced by* k *vertices,* $3 \leq k \leq n$ *such that,* *(i) if k is even, the labels of the k vertices are $\{i+1, i+2, \cdots, i+k\}$ and*

(ii) if k is odd, the labels of $k-1$ vertices are $\{i+1, i+2, \cdots, i+k-1\}$ and the k^{th} vertex is labeled $i-1, i, i+k$, or $i+k+1$

where i is odd and the labels are taken modulo $2n$. Then H is a maximum subgraph of $P(n,1), n \geq 3$.

Complete binary trees are perfectly balanced and have the maximum possible number of nodes, given their height. However, they exist only when n is one less than a power of 2. For any non-negative integer n, the complete binary tree of height n, denoted by T_n, is the binary tree where each internal vertex has exactly two children and all the leaves are at the same level. Thus a complete binary tree T_n has n levels and level i, $i \leq i \leq n$, contains $2^i - 1$ vertices. Thus T_n has exactly $2^n - 1$ vertices.

Definition 3.27 [18] *The 1-rooted complete binary tree T_n^1 is obtained from a complete binary tree T_n by attaching to its root a pendant edge. The new vertex is called the root of T_n^1 and is considered to be at level 0. The k-rooted complete binary tree T_n^k is obtained by taking k vertex disjoint 1-rooted complete binary trees T_n^1 on 2^n vertices with roots say $r_1, r_2, \cdots, r_k$ and adding the edges $(r_i, r_{i+1}), 1 \leq i \leq k-1$. See Figure 7(a).*

Theorem 3.28 *The exact wirelength of embedding a generalized Petersen graph $P(2^{n-1}, 1)$ into the 1-rooted complete binary tree T_n^1 is given by,*

$$WL(P(2^{n-1},1), T_n^1) = 27(2^{n-3}) + 3 + \sum_{j=4}^{n-1} 2^{n-j}[3(2^j-1) - 2(2^j + \lfloor \frac{2^j-1}{2} \rfloor - 3)]$$

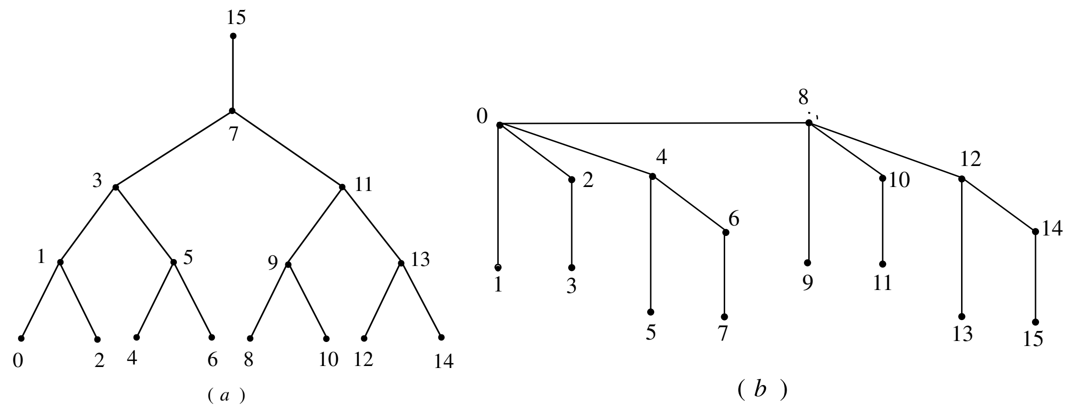

Figure 7: (a)1-rooted complete binary tree with inorder labeling, (b) Binomial tree B_4

Theorem 3.29 *The exact wirelength of embedding a generalized Petersen graph $P(2^{n-1},1)$ into the k-rooted complete binary tree $T^k_{n_1}$ is given by,*

$$\begin{aligned} WL(P(2^{n-1},1),T^k_{n_1}) &= 27(2^{n-3})+3+\sum_{j=4}^{n-1}2^{n-j}[3(2^j-1)-2(2^j+\lfloor\frac{2^j-1}{2}\rfloor-3)] \\ . \quad & +4(k-1) \end{aligned}$$

Definition 3.30 [18] *A binomial tree B_0 of height 0 is a single vertex. For all $n>0$, a binomial tree B_n of height n is a tree formed by joining the roots of two binomial trees of height $n-1$ with a new edge and designating one of these roots to be the root of the new tree. A binomial tree of height n has 2^n vertices. See Figure 7(b).*

Theorem 3.31 *The exact wirelength of embedding a generalized Petersen graph $P(2^{n-1},1)$ into the binomial tree B_n is given by,*

$$WL(P(2^{n-1},1),B_n) = 3(2^{n-1})+4+\sum_{j=2}^{n-1}2^{n-j}[3(2^{j-1})-2^j-2^{j-1}+4].$$

The contents of this chapter has been *submitted* to the **Journal of Computer Science.**

In Chapter 7, we determine the PI Index of Mesh Structured Chemicals.

Graph theory represents a very natural formalism for chemistry and has already been employed in a variety of implicit forms. Its applications began to multiply so fast that chemical graph theory bifurcated in manifold ways to evolve into an assortment of different specialisms. The current panorama of chemical graph theory has been erected on foundations that are essentially graph-theoretical in nature. The chemical graphs are now being used for many different purposes in all the major branches of chemical engineering and this renders the origin of the earliest implicit application of graph theory of some considerable interest. The mesh, honeycomb and diamond networks are not only important interconnection networks but also bear resemblance to atomic or molecular lattice structures of chemical compounds. A survey of these networks is given in [36]. There are three possible tessellations of a plane with regular polygons of the same kind: square, triangular and hexagonal, corresponding to dividing a plane into regular squares, triangles and hexagons respectively. The mesh network is based on square tessellation whereas the honeycomb mesh is based on hexagonal tessellation.

We compute the PI index of mesh, torus and honeycomb mesh networks making use of embedding techniques. Further, we also derive the PI index of $NaCl$ molecule.

Lemma 3.32 *The PI index of a graph $G(p,q)$ is given by $PI = q^2 - \sum_{e \in E} |\tau_e|$, where q is the number of edges in G and for any edge $e = (u,v), \tau_e$ is the set of edges which are equidistant from both u and v.*

Lemma 3.33 *Let $G = (V,E)$ be a graph and let $\{E_1, E_2, \cdots, E_k\}$ be a partition of E such that for, $e, e' \in E_i, 1 \leq i \leq k, \tau_e = \tau_{e'}$ then $PI(G) = q^2 - \sum_{i=1}^{k} |\tau_{e_i}| t_i$ where $t_i = |E_i|$*

and $e_i \in E_i, 1 \leq i \leq k$.

Theorem 3.34 *The* PI *index of the 3-dimensional mesh* $M(r,s,t)$ *is given by* $PI(M(r,s,t)) = (3rst - (rs + st + tr))^2 - (r-1)s^2t^2 - (s-1)t^2r^2 - (t-1)r^2s^2$.

Theorem 3.35 *The* PI *index of the sodium chloride* $NaCl$ *is given by* $PI(NaCl) = 2430$.

Theorem 3.36 *The PI index of the torus* $T(m,n)$ *is given by,*

$$PI(T(m,n)) = \begin{cases} 2mn(2mn - m - n), & \textit{when m,n are even;} \\ mn(4mn - m - n), & \textit{when m,n are odd;} \\ mn(4mn - m - 2n), & \textit{when m is even and n is odd;} \\ mn(4mn - 2m - n), & \textit{when m is odd and n is even.} \end{cases}$$

Theorem 3.37 *The* PI *index of the honeycomb mesh* HM_d *of dimension* d*, is given by* $PI(HM_d) = (9d^2 - 3d)^2 - 12d^2 - 6\sum_{i=1}^{d-1}(2d-i)^2$.

Theorem 3.38 *The* PI *index of benzenoid graph* $G(m,n)$ *is given by*

$$PI(G(m,n)) = \begin{cases} 8m^2 + 24n^2 + 30mn + 10n + 2, & \textit{n > m;} \\ 62n^2 + 26n + 8, & \textit{n = m.} \end{cases}$$

The results obtained in this chapter have been presented in The International Conference on Informatics Engineering and Information Science (ICIEIS 2011), Malaysia November 14-16, 2011. Also, these results have been **published** in: Proceedings of ICIEIS 2011, **Lecture Notes in Computer Science**, Springer-Verlag, CCIS 253, no. 3, 400–409, 2011.

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