Symmetric Interconnection Networks from Cubic Crystal Lattices

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Abstract

Torus networks of moderate degree have been widely used in the supercomputer industry. Tori are superb when used for executing applications that require near-neighbor communications. Nevertheless, they are not so good when dealing with global communications. Hence, typical 3D implementations have evolved to 5D networks, among other reasons, to reduce network distances. Most of these big systems are mixed-radix tori which are not the best option for minimizing distances and efficiently using network resources. This paper is focused on improving the topological properties of these networks.

By using integral matrices to deal with Cayley graphs over Abelian groups, we have been able to propose and analyze a family of high-dimensional grid-based interconnection networks. As they are built over n-dimensional grids that induce a regular tiling of the space, these topologies have been denoted lattice graphs. We will focus on cubic crystal lattices for modeling symmetric 3D networks. Other higher dimensional networks can be composed over these graphs, as illustrated in this research. Easy network partitioning can also take advantage of this network composition operation. Minimal routing algorithms are also provided for these new topologies. Finally, some practical issues such as implementability and preliminary performance evaluations have been addressed.

1 Introduction

Interconnection networks are critical subsystems in modern supercomputers. Currently, the top 5 supercomputers composed of Cray XK7, IBM BluGene/Q and K computers, use moderate degree networks. The Cray employs a 3D torus whereas BlueGene uses a 5D one, [14, 12]. The K computer employs small 3D meshes (that can also be seen as 4 × 3 tori) connected by a bigger 3D torus [1]. All these topologies are mixed-radix torus, as they have dimensions of different sizes. For example, a configuration for a Cray Jaguar can be 25 × 32 × 16 and a BlueGene configuration 16 × 16 × 16 × 12 × 2. The 88,128-node K computer installed at Riken, is compatible with a 17 × 18 × 24 torus connecting 3D meshes of 12 nodes. Mixed-radix tori are not edge-symmetric, which can lead to unbalanced use of their network links. However, these big systems are typically divided into smaller partitions which enables them to be used by multiple users. Hence, providing symmetry, at least, in typical network partitions is an advisable design goal.

Tori are not well suited to support global and remote communications. Their relatively long paths among nodes, especially their diameter and average distance, incur high latencies and reduced throughput. Thus, reducing topological distances in the network should be pursued. The way to achieve network distance reductions is by changing the topology. Topological changes depend on the router degree. If the router degree must be kept within the current values, it would be interesting to preserve the good topological properties of tori such as grid locality, easy partitioning and simple routing. Hence, practicable topological changes should not be radical. A typical technique employed to this end has been twisting the wrap-around links of tori, [3, 27, 4, 20]. Interestingly, this twisting also allows for edge-symmetric networks of sizes for which their corresponding tori are asymmetric, [7, 9]. Twisting 2D tori is nearly as old as the history of supercomputers. The Illiac IV developed in 1971 already employed a twisted network. Many works dealing with twisted 2D tori have been published since then. However, when scaling dimensions, the problem of finding a good twisting scheme becomes harder. Very few solutions are known for 3D, with the one presented in [7] being a practicable example. Exploring the effect of twists in higher dimensions remains, to our knowledge, an unexplored domain. If the router degree can be increased, a radically different solution for reducing network diameter can be used in high-degree hierarchical networks, [15]. These direct networks employing high-degree routers are beyond the scope of this paper.

It has been recognized for a long time that Cayley graphs are well suited to interconnection networks. Actually, the widely used rings and tori are Cayley graphs. Nowadays, rings are common in on-chip networks [25] and, as stated previously, tori dominate high-end supercomputing. In [16], Fiol introduced multidimensional circulant graphs as a new algebraic representation for Cayley graphs over Abelian groups. This representation has proved its suitability for studying and characterizing 2D grid-based networks in [9]. In this paper, lattice networks are introduced as multidimensional circulants with orthonormal adjacencies, that is, multidimensional grids plus additional wrap-around links which complete their regular adjacency. Therefore, this work is devoted to the study of high dimensional twisted tori topologies. Although special attention will be devoted to symmetric 3D networks, higher dimensional topologies which em-
bed these symmetric 3D networks will also be considered. Specifically, the main contributions of this paper are:

- A characterization of 3D symmetric networks which correspond to cubic crystal lattices.
- A general method for lifting crystal graphs which leads to higher dimensional lattice networks that embed crystal networks.
- A minimal routing mechanism that performs over any lattice network.
- A first approach to practical issues such as implementability and a preliminary performance evaluation of these networks, which includes both topological models and empirical simulations.

The remainder of this paper is organized as follows. Section 2 defines lattice graphs, introduces the concepts of graph lift and projection and provides some network examples. Section 3 focuses on 3D networks, describes symmetric cubic crystal graphs and performs a topological comparison of these networks with standard mixed-radix tori. Section 4 introduces two methods for scaling crystal networks to higher dimensions and presents some examples. Section 5 presents minimal routing algorithms for lattice networks. Section 6 discusses implementability and performance issues. Finally, Section 7 concludes the paper summarizing its main findings.

## 2 Lattice Graphs

In this section we introduce lattice graphs which will be used to model interconnection networks of any finite dimension. The lattice graph is not a new concept, in fact, it has many different uses. The most extensively used, which is the one used in this paper, is as a graph built over an \( n \)-dimensional grid which induces a regular tiling of the space. On the other hand, lattice graphs also appear in the literature under other names for example, tiling graphs. Moreover, in \[16\], multi-dimensional circulants were defined as lattice graphs but for smaller dimensions which are embedded in it, while lifting a lattice graph will be used for increasing its dimension.

Lattice graphs are defined over the integer lattice \( \mathbb{Z}^n \). A lattice graph will be used for increasing its dimension. Projecting a lattice graph allows the study of the different lattice graphs of smaller dimensions which are embedded in it, while lifting a lattice graph will be used for increasing its dimension.

Lattice graphs are defined over the integer lattice \( \mathbb{Z}^n \). Hence, their nodes are labelled by means of \( n \)-dimensional (column) integral vectors. A lattice graph can be intuitively seen as a multidimensional grid with additional wrap-around links completing the regular adjacency. Before proceeding with their formal definition, first we introduce some notation.

### Notation 1
The following notation will be used throughout the article:

- Lower case letters denote integers: \( a, b, \ldots \)
- Bold font denotes integer column vectors: \( \mathbf{v}, \mathbf{w}, \ldots \)
- Capitals correspond to integer matrices: \( M, P, \ldots \)
- \( \mathbf{e}_i \) denotes the vector with a 1 in its \( i \)-th component and 0 elsewhere.
- \( B_n = \{ \mathbf{e}_i \mid i = 1, \ldots, n \} \) denotes the \( n \)-dimensional orthonormal basis.

To define the finite set of nodes of these graphs and their wrap-around links, a modulo function using a square integer matrix will be used. Hence, congruences modulo matrices are introduced in the next definition.

### Definition 2
\[16\] Let \( M \in \mathbb{Z}^{n \times n} \) be a non-singular square matrix of dimension \( n \). Two vectors \( \mathbf{v}, \mathbf{w} \in \mathbb{Z}^n \) are congruent modulo \( M \) if and only if we have \( \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} \in \mathbb{Z}^n \) such that:

\[
\mathbf{v} - \mathbf{w} = u_1 \mathbf{m}_1 + u_2 \mathbf{m}_2 + \cdots + u_n \mathbf{m}_n = M \mathbf{u}
\]

where \( \mathbf{m}_j \) denotes the \( j \)-th column of \( M \). We will denote this congruence as \( \mathbf{v} \equiv \mathbf{w} \pmod{M} \).

The set of nodes of a lattice graph will be the elements of the quotient group

\[
\mathbb{Z}^n / M \mathbb{Z}^n = \{ \mathbf{v} \pmod{M} \mid \mathbf{v} \in \mathbb{Z}^n \}
\]

generated by the equivalence relation induced by \( M \). As was proved in \[16\], \( \mathbb{Z}^n / M \mathbb{Z}^n \) has \( |\det(M)| \) elements. Now, we can proceed with a formal definition of a lattice graph.

### Definition 3
Given a square non-singular integral matrix \( M \in \mathbb{Z}^{n \times n} \), we define the lattice graph generated by \( M \) as \( G(M) \), where:

i) The vertex set is \( \mathbb{Z}^n / M \mathbb{Z}^n = \{ \mathbf{v} \pmod{M} \mid \mathbf{v} \in \mathbb{Z}^n \} \).

ii) Two nodes \( \mathbf{v} \) and \( \mathbf{w} \) are adjacent if and only if \( \mathbf{v} - \mathbf{w} \equiv \pm \mathbf{e}_i \pmod{M} \) for some \( i \in \{ 1, \ldots, n \} \).

From here onwards, all matrices will be considered to be non-singular, unless the contrary is stated. Note that, since \( \mathbb{Z}^n / M \mathbb{Z}^n \) has \( |\det(M)| \) elements, this will be the number of nodes of \( G(M) \). Moreover, since any vertex \( \mathbf{v} \) is adjacent to \( \mathbf{v} \pm \mathbf{e}_i \pmod{M} \), the lattice graph \( G(M) \) is regular of degree \( 2n \), that is, any node has \( 2n \) different neighbours. As stated in the following two paragraphs, tori are lattice graphs.
Definition 4. The n-dimensional torus graph of sides \( a_1, \ldots, a_n \), denoted by \( T(a_1, \ldots, a_n) \) is defined as a graph with vertices \( x \in \mathbb{Z}^n \) such that \( 0 \leq x_i < a_i \). Two vertices \( x \) and \( y \) are adjacent if and only if they differ in exactly one coordinate, let us say \( i \), for which \( x_i \equiv y_i \pm 1 \) (mod \( a_i \)).

Theorem 5. The torus graph \( T(a_1, \ldots, a_n) \) is isomorphic to the lattice graph \( G(\text{diag}(a_1, \ldots, a_n)) \), where \( \text{diag}(a_1, \ldots, a_n) \) denotes the square diagonal matrix with diagonal equal to \( a_1, \ldots, a_n \).

Proof. Clearly the vertex space of both graphs is the same. In the following we check that adjacencies are preserved. If \( x \) is connected to \( y \) then it holds that \( y - x = (y_i - x_i)e_i \). Then for some integer \( k \), \( y - x = (\pm 1 + ka_i)e_i = \pm e_i + ka_i e_i = \pm e_i + \text{diag}(a_1, \ldots, a_n)ke_i \). Hence \( y - x \equiv \pm e_i \) (mod diag\((a_1, \ldots, a_n)\)). \( \square \)

Next we recall some known results from [10] about right-equivalent matrices.

Definition 6. \( M_1 \) is right equivalent to \( M_2 \), which is denoted by \( M_1 \cong M_2 \), if and only if there exists a unitary matrix \( P \in \mathbb{Z}^{n \times n} \) such that \( M_1 = PM_2P^{-1} \).

As was proved in [10], if \( M_1 \cong M_2 \) then the graphs \( G(M_1) \) and \( G(M_2) \) are isomorphic. As a consequence, performing Gaussian elimination by columns in the generating matrix gives isomorphic graphs. After one phase of Gaussian elimination we obtain:

\[
M \cong \begin{pmatrix} B & c \\ 0 & a \end{pmatrix}
\]

where \( B \in \mathbb{Z}^{n-1 \times n-1} \) is a matrix of smaller dimension, \( c \in \mathbb{Z}^{n-1} \) is a column vector and \( a \) is a positive integer. As a consequence, we obtain that \( |\det(M)| = |\det(B)|a \), that is, the order of \( G(M) \) can be expressed in terms of \( G(B) \) and the integer \( a \). Moreover, the lattice graph \( G(B) \) is isomorphic to the subgraph of \( G(M) \) generated by \( \{ \pm e_1, \pm e_2, \ldots, \pm e_{n-1} \} \), which allows us to state the following definition.

Definition 7. Let \( M \in \mathbb{Z}^{n \times n} \) be non-singular and \( G(M) \) be its lattice graph. Let us consider \( M \cong \begin{pmatrix} B & c \\ 0 & a \end{pmatrix} \) such that \( a \) is a positive integer. Then, we will say that \( a \) is the side of \( G(M) \) and \( G(B) \) its projection over \( e_n \). Moreover, we will call \( G(M) \) a lift of \( G(B) \).

In particular, any lattice graph can be considered to be generated by its unique Hermite matrix, which may be convenient as Examples 9 and 10 attempt to demonstrate. Before stating the examples, we recall the Hermite normal form of a matrix.

Definition 8. A matrix \( H \) is said to be in Hermite normal form if it is upper triangular, has positive diagonal and each \( H_{i,j} \) with \( j > i \) lies in a complete set of residues modulo \( H_{i,i} \).

Definitions 7 and 8 allow us to consider a helpful graphical visualization of any lattice graph which will also be used for routing in Section 5. First, lattice graphs and their subgraphs can be seen as n-dimensional spaces whose dimensions are sized by the elements in the principal diagonal of \( M \). Each column vector in \( M \) represents a graph dimension, signaling the point in the space at which a new copy of the tile induced by \( M \) is located; this is important as column vectors dictate the pattern of the wrap-around connections of each dimension.

Moreover, from the cardinal equality \( |G(M)| = |G(B)|a \), the lattice graph \( G(M) \) can be seen as composed of a disjoint copies of its projection \( G(B) \). One or several parallel cycles connect these disjoint copies completing the adjacency pattern. The length of these cycles can be computed as \( \text{ord}(e_n) \), which is the order of the element \( e_n \) in the group \( \mathbb{Z}^n/M\mathbb{Z}^n \). According to [10], the order of any element \( x \) can be computed as

\[
\frac{\det(M)}{\text{gcd}(\det(M), \text{gcd}(\det(M), M^{-1}x))}.
\]

Note that the second gcd (greatest common divisor) in the fraction corresponds to the gcd of the elements of a vector. The number of vertices of each cycle lying in each copy of \( G(B) \) can be calculated as the length of the cycle over the side of the graph, that is \( \frac{\text{ord}(e_n)}{a} \).

Example 9. Let us consider the rectangular twisted torus of size \( 2a \times a \) and twist \( a \), denoted as \( \text{RTT}(a) \) in [7]. This graph can be seen to be generated by the matrix \( H = \begin{pmatrix} 2a & a \\ 0 & a \end{pmatrix} \). Using \( H \), the graph can be seen as a grid of \( 2a \times a \) \((h_{1,1} \times h_{2,2})\). Wrap-around links in \( e_1 \) (first) dimension conserve their horizontality since \( h_{2,1} = 0 \); wrap-around links in \( e_2 \) (second) dimension do not conserve their verticality but suffer a twist of a column since \( h_{1,2} = a \). According to Definition 7, the projection over \( e_2 \) of \( \text{RTT}(a) \) is a cycle of 2a nodes each. As the side of \( \text{RTT}(a) \) is a, it will have a disjoint cycles of 2a nodes. As \( \text{ord}(e_2) \) (the element representing a jump in \( e_2 \) dimension) is \( 2a \), the graph will have a parallel cycles of length 2a in that dimension. Each of these a cycles contains two vertices of each projection. A graphical representation of \( \text{RTT}(4) \) can be seen in Figure 4.

Example 10. Let us now consider the lattice graph \( G(M) \) with \( M = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 2 \\ 0 & 0 & 4 \end{pmatrix} \). Note that \( M \) is in Hermite form. \( G(M) \) can be seen as a 4 x 4 x 4 cubic grid. Three sets of wrap-around links, each one connecting opposite faces, have to be added to the grid-based cube. Wrap-around links in \( e_1 \) always remain horizontal by construction, as imposed by the \( n-1 \) zeros in the first column vector of any Hermite matrix. Wrap-around links in \( e_2 \) dimension remain vertical in this graph because \( n_{1,2} = 0 \) but, in general, they can undergo only a twist over the \( e_1 \) dimension of \( n_{1,2} \) units.
Finally, wrap-around links in the \( e_3 \) dimension can undergo twists over both \( e_1 \) and \( e_2 \) dimensions. In the graph of this example, no twist is applied in \( e_3 \) over \( e_1 \) because \( m_{1,3} = 0 \) and a twist of 2 units is applied over the \( e_2 \) dimension as \( m_{2,3} = 2 \). As can be seen in Figure 2, the projection of \( G(M) \) is a 2D torus \( T(4,4) \). Thus, the graph is composed of 4 disjoint copies of its projection, each of them connected by a cycle of length 8, as represented in the figure. Note that for every vertex in the graph there will be a similar cycle with the same pattern as the one represented in the figure. The cycle intersects in two vertices with each copy of the projection. For the sake of the clarity, only one cycle between copies of \( G(4,0) \) has been represented.

Figure 1: Two perpendicular cycles of length 8 in the RTT(4).

Figure 2: The cycle \( \langle e_1 \rangle \) joining by the disjoint copies of the projection.

Note that we can project over any \( e_i \), simply by swapping rows \( i \) and \( n \) (which gives an automorphic graph) and then, project over \( e_n \). Moreover, as we will see later, symmetries will make irrelevant over which dimension we project, so we will consider \( e_n \) by default. The resulting projection can again be projected over another vector, which results in a projection over a plane of the lattice graph. Clearly, projecting over a pair of vectors \( \{ e_i, e_j \} \) can be done in any order, since projecting first over \( e_i \) and then over \( e_j \) results in the same graph as projecting first over \( e_j \) and then over \( e_i \). Following the same idea, we can project over several dimensions iteratively. Therefore, we will call the result of projecting iteratively over the vectors in the set \( \{ e_1, \ldots, e_n \} \) the projection of \( G(M) \) over the set. In this case we will call it a \( r \)-dimensional projection which turns into a lattice graph generated by a \((n-r) \times (n-r)\) matrix.

### 3 Cubic Crystal Graphs

Symmetry is a desirable property for any network as it impacts on performance and routing efficiency. Many interconnection networks have been based on vertex-symmetric graphs, but less attention has been devoted to edge-symmetric networks. Square and cubic tori have been the networks of choice for many designs as they are symmetric (vertex and edge symmetric). For this reason, symmetric lattice graphs will be considered in this section. Hence, we next introduce the concept of a symmetric graph.

A graph \( G = (V, E) \) is vertex-symmetric (or vertex-transitive) if for each pair of vertices \((x, y) \in V \), there is an automorphism \( \phi \) of \( G \) such that \( \phi(x) = y \). Also, \( G \) is edge-symmetric (or edge-transitive) if for each pair of edges \( \{x_1, x_2\}, \{y_1, y_2\} \in E \), there is an automorphism \( \phi \) of \( G \) such that \( \phi(\{x_1, x_2\}) = \{\phi(x_1), \phi(x_2)\} = \{y_1, y_2\} \). Finally, \( G \) is said to be symmetric when it is both vertex-symmetric and edge-symmetric. Since every Cayley graph is vertex-symmetric [2], we will focus on edge-symmetry. As was shown in [8], the consideration of non-linear automorphisms in the edge-symmetry characterization leads to marginal families of graphs which do no exemplify the general behaviour. Hence, in this paper we will refer only to automorphisms which are linear applications. Therefore, in an abuse of notation, symmetric graphs will refer to those in which there exist a linear automorphism fulfilling the previous definition.

**Theorem 11.** The projections of a symmetric lattice graph are all isomorphic.

**Proof.** Let us denote \( proj_i(G(M)) \) to be the projection of \( G(M) \) over \( e_i \). We know \( proj_i(G(M)) \) is isomorphic to the subgraph of \( G(M) \) generated by \( B_n \setminus \{ e_i \} \). As \( G(M) \) is symmetric we know \( \phi \in Aut(G(M)) \) such that \( \phi(e_i) = \pm e_j \). As \( e_i \) is the only generator not in \( proj_i(G(M)) \), \( e_j \) is the only generator not in \( \phi(proj_i(G(M))) \). Hence, as \( \phi \) is an automorphism, we deduce that \( proj_i(G(M)) \cong proj_j(G(M)) \).

Now, we concentrate on 3D symmetric graphs. In Appendix I it is proved that the only symmetric 3D lattice graphs are the ones given by the matrices described in the next result.
Theorem 12. Let $M \in \mathbb{Z}^{3 \times 3}$. Then, the lattice graph $\mathcal{G}(M)$ is symmetric if and only if it is isomorphic to $\mathcal{G}(M')$ where:

$$M' \in \left\{ \begin{pmatrix} a & c & b \\ b & a & c \\ c & b & a \end{pmatrix}, \begin{pmatrix} a & b & c \\ a & c & -b - c \\ -a & b & a \end{pmatrix} \right\}.$$ 

The previous characterization gives us a broad family of symmetric graphs. However, there are matrices belonging to the first case that deserve special attention, such as the ones that generate the cubic crystal lattices, which are:

- **Primitive Cubic Lattice:** $\begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix}$.

- **Face-centered Cubic Lattice:** $\begin{pmatrix} a & a & 0 \\ a & 0 & a \\ 0 & a & a \end{pmatrix}$.

- **Body-centered Cubic Lattice:** $\begin{pmatrix} -a & a & a \\ a & -a & a \\ a & a & -a \end{pmatrix}$.

In the following subsections we will consider the lattice graphs defined by cubic crystal lattices, their isomorphisms with previously studied network topologies and a comparison among them in terms of their distance properties.

### 3.1 Primitive Cubic lattice graph

We define the Primitive Cubic Lattice Graph $PC(a)$ as the lattice graph generated by the matrix associated with the primitive cubic lattice, that is:

$$\begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix}.$$ 

Clearly, the order of the graph is $a^3$, which is the determinant of the diagonal matrix. According to Theorem 5, $PC(a)$ is isomorphic to the 3D torus of side $a$, or equivalently, the $a$-ary 3-cube.

Lemma 13. The projection of $PC(a)$ is the 2D torus graph of side $a$ or $\mathcal{G}\left( \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \right)$.

### 3.2 Face-centered Cubic lattice graph

The Face-centered Cubic lattice graph $FCC(a)$ of side $a$ can be defined as the lattice graph generated by the matrix associated with the face-centered cubic crystal lattice, that is:

$$\begin{pmatrix} a & a & 0 \\ a & 0 & a \\ 0 & a & a \end{pmatrix} \cong \begin{pmatrix} 2a & a & a \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix}.$$ 

The order of the graph is $|\det(M)| = 2|a|^3$.

### 3.3 Body-centered Cubic lattice graph

The Body-centered Cubic lattice graph $BCC(a)$ of side $a$ can be defined as the lattice graph generated by the matrix:

$$\begin{pmatrix} -a & a & a \\ a & -a & a \\ a & a & -a \end{pmatrix} \cong \begin{pmatrix} 2a & 0 & a \\ 0 & 2a & a \\ 0 & 0 & a \end{pmatrix}.$$ 

The order of the graph is $4a^3$. As far as we know, this graph has not previously been considered for interconnection networks. However, as we will see later, the graph not only meets the symmetry requirements but also has a good order/diameter correspondence. Moreover, it embeds 2D symmetric tori as is proved in:

Lemma 16. The projection of $BCC(a)$ is the 2D torus graph $T(2a, 2a)$.

Theorem 14. The projection of $FCC(a)$ is the rectangular twisted torus graph of side $a$, $RTT(a)$.

Proof. After performing Gaussian elimination, on the right of the previous expression we obtained the Hermite form of the matrix. It is easy to see that its projection is generated by $\begin{pmatrix} 2a & a \\ 0 & a \end{pmatrix}$. As we have seen before and was proved in [9], this graph is isomorphic to the rectangular twisted torus $RTT(a)$ of side $a$ or the Gaussian graph generated by $a + ai$ [22].

A $FCC(a)$ is isomorphic to the prismatic doubly twisted torus of side $a$ ($PDTT(a)$), introduced in [7], as the next proposition proves.

Proposition 15. $FCC(a)$ is isomorphic to the prismatic doubly twisted torus of side $a$, $PDTT(a)$.

Proof. The $PDTT(a)$ was defined in [7] as a graph in which the connectivity of each plane is a $RTT(a)$, hence the isomorphism is immediate once we have proved that all the projections of $FCC(a)$ are isomorphic to $RTT(a)$. Note that this fact can be inferred from Lemma 14 and Theorem 11.

### 3.4 Cubic crystal lattice graph comparison

In previous subsections, three different 3D symmetric topologies based on cubic crystal lattices have been introduced. As we have seen, two of them—the 3D torus or $PC$ and the PDTT or $FCC$—were previously known, and the last one, that is the $BCC$, is a new proposal introduced in this paper. In this subsection, our aim is to consider...
their distance properties and to perform a first comparison in terms of diameter, average distance and projections.

First of all, we would like to highlight that a cubic crystal lattice graph exists for any order that is a power of two. This is important because we can gracefully upgrade a network in three steps while conserving symmetry. If \( t \) is a positive integer, then:

- There exists a primitive cubic lattice graph with \( 2^{3t} \) nodes.
- There exists a face-centered cubic lattice graph with \( 2^{3t+1} \) nodes.
- There exists a body-centered cubic lattice graph with \( 2^{3t+2} \) nodes.

Although this fact provides practical versatility, it complicates the comparison among networks. The exact expressions for average distance of the three crystals are given next:

- \( \text{PC}(a) \) has average distance:
  \[
  \bar{k} = \begin{cases} 
    \frac{3a^4}{3(a^3-1)} & \text{if } 2|a \\
    \frac{3a^6-3a^2}{4(a^3-1)} & \text{if } 2 \nmid a 
  \end{cases}
  \]

- \( \text{FCC}(a) \) has average distance:
  \[
  \bar{k} = \begin{cases} 
    \frac{7a^4-2a^2}{4(2a^3-1)} & \text{if } 2|a \\
    \frac{7a^6-2a^2-1}{4(2a^3-1)} & \text{if } 2 \nmid a 
  \end{cases}
  \]

- \( \text{BCC}(a) \) has average distance:
  \[
  \bar{k} = \begin{cases} 
    \frac{35a^4-8a^2}{8(4a^3-1)} & \text{if } 2|a \\
    \frac{35a^6-14a^2+30}{8(4a^3-1)} & \text{if } 2 \nmid a 
  \end{cases}
  \]

These expressions have been calculated under the assumption that the average distance fulfills a polynomial expression, which is a reasonable hypothesis. Moreover, these values have been computationally checked for orders up to 40,000. In Table I the distance properties for the three graphs are summarized. For an easier comparison, note that average distance values are given as approximations. Mixed-radix torus graphs which have the same number of nodes of the \( \text{FCC} \) and \( \text{BCC} \) crystals have been also added in the table. Clearly, the crystals have better distance properties than their corresponding torus networks. Moreover, \( \text{BCC} \) is more dense than the other two cubic crystals since, for the same diameter, it attains a greater number of nodes.

Finally, as we have seen in previous subsections, while \( \text{FCC} \) has the twisted torus as its projection, both \( \text{PC} \) and \( \text{BCC} \) are lifts of a 2D symmetric torus graph.

Having considered distance-related parameters for comparing crystals, let us also take into account other topological parameters to complete the study. In networking literature, the \textit{bisection bandwidth} (BB) is used to obtain an upper bound for the network load under uniform random traffic. However, it was shown in [7] that in rectangular twisted tori some minimal routes between pairs of vertices in opposite network partitions could traverse the bisection twice. Hence, this work proved that \( BB \) is not a tight bound for network throughput in twisted topologies. Indeed, the same happens with any non-torus lattice graph.

Table 1: Distance properties of cubic crystal lattice graphs.
throughput under uniform traffic under ideal conditions. Throughput is inversely proportional to average distance in symmetric networks. As, under uniform traffic at rate \( l \), \( l \) phits are injected into each node each cycle, we have a total of \( lNk \) links being used each cycle. As a link can only transfer 2 phits (one in each way) each cycle, we have \( lNk \leq 2|E| = \Delta N \), where \( \Delta \) denotes the graph degree and \( N \) and \( E \) denote the order and the edge set respectively. Thus, network throughput is bounded by \( \frac{\Delta}{k} \); for lattice graphs, \( \Delta = 2n \) where \( n \) is the number of dimensions. Hence, FCC(a) maximum throughput will be bounded by \( \frac{48}{7a} \) and BCC(a) by \( \frac{192}{35a} \). Nevertheless, the previous count cannot be applied to edge-asymmetric networks such as mixed-radix tori. In that case, it can be seen that throughput is inversely proportional to the maximum average distance per dimension, namely \( \frac{\Delta}{nk_{max}} \), as inferred from [7].

Network throughput for both \( T(2a, a, a) \) and \( T(2a, 2a, a) \) is bounded by \( \frac{12}{3a} = \frac{4}{a} \) as \( k_{max} \approx \frac{a}{2} \), given that their longest dimensions are \( 2a \)-node rings. This leads to an improvement in maximum throughput under uniform traffic of 71% when comparing FCC(a) to \( T(2a, a, a) \) and 37% for BCC(a) versus \( T(2a, 2a, a) \).

Being symmetric has more positive impact when the number of nodes is \( 2a^3 \). In \( T(2a, a, a) \), when the links in the longest dimension are fully utilized, links in the other two shortest dimensions are used at 50%. This is because, on average, the length of the paths in the longest dimension doubles the length of the shortest ones. When the number of nodes is \( 4a^3 \), \( T(2a, 2a, a) \) uses its resources better as only links in one dimension operate at half rate.

### 4 Higher Dimensions: Lifts and Hybrid Graphs

In the previous section we characterized 3D symmetric topologies and detailed the special case of the cubic crystal graphs. Symmetry could help when the application runs on the whole network. However, in big systems the user typically only has a partition of the complete machine assigned. Therefore, looking for symmetry in higher dimensions cannot be prioritized. Nevertheless, reducing the distance properties of the whole network would be still beneficial since applications and system software sometimes run over the entire network. Consequently, what we look for are higher dimensional networks embedding the previous crystal cubic lattice graphs.

In the next subsections we explore two different methods for upgrading the previous cubic crystal lattice graphs. In the first subsection, we consider the lifting of crystal graphs, which results in 4D topologies. Whenever possible, the lift is done in such a way that the resulting eight-degree topology preserves symmetry. To end this subsection, we will introduce a tree that represents the process of network upgrading, preserving symmetry. In the second subsection we present common lifts of lattice graphs. The ultimate aim of this new method is to build new lattice graphs which embed other lattice graphs, while minimizing the necessary network degree to obtain them. The resulting graphs have been denoted as hybrid graphs since several lattice graphs of different nature (symmetric or non-symmetric) and degrees are embedded on them.

#### 4.1 Symmetric Lifts of Cubic Crystal Graphs

First, we consider the \( PC \). There is a straightforward way of lifting a PC(a) to 4D, which is the Cartesian product of the PC by one cycle of length \( a \), thus obtaining the generator matrix:

\[
\begin{pmatrix}
a & 0 & 0 & 0 \\
0 & a & 0 & 0 \\
0 & 0 & a & 0 \\
0 & 0 & 0 & a \\
\end{pmatrix}
\]

The 4D torus generated by the previous matrix is completely symmetric. However, the lifting technique can be used to embed the completely symmetric 3D torus in a different lattice graph. We will denote the body centered hypercube lattice graph as 4D-BCC, that is, the lattice graph generated by matrix:

\[
\begin{pmatrix}
2a & 0 & 0 & a \\
0 & 2a & 0 & a \\
0 & 0 & 2a & a \\
0 & 0 & 0 & a \\
\end{pmatrix}
\]

**Proposition 17.** 4D-BCC(a) is a symmetric lattice graph of side \( a \) and projection PC(2a).

**Proof.** Let \( \phi \) be defined by \( \phi(e_i) = e_{i+1} \) (mod \( n \)). \( \phi \) has an associated matrix \( P = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \). As \( Q = M^{-1}PM = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 2 & 1 \end{pmatrix} \) is an integer matrix we conclude that \( \phi \) is an automorphism of 4D-BCC [8]. In the group generated by \( \phi \) there are enough automorphisms to provide the edge-symmetry. It should be noted that the projection is straightforward as the matrix is triangular superior.

Now, if we want to lift the FCC, there are two ways of doing so which make the lifted graph symmetric. The first one will be denoted as 4D-FCC (4-dimensional face-centered cubic lattice graph), that is, the lattice graph generated by matrix:
Proposition 17. \(4D-FCC(a)\) is a symmetric lattice graph of side \(a\) whose projection is a FCC(a).

Proof. Exactly like the proof of Proposition \ref{prop:lempg} the matrix \(Q = M^{-1}PM\) is different but still with integer entries. \(\blacksquare\)

The second way to lift FCC is introduced below.

Proposition 19. The lattice graph generated by the matrix
\[
\begin{pmatrix}
a & -a & -a & -a \\
a & a & -a & -a \\
a & a & a & -a \\
a & -a & a & a
\end{pmatrix}
\]
is a symmetric lifting of the FCC(2a).

Proof. The isomorphism is guaranteed since
\[
\begin{pmatrix}
a & -a & -a & -a \\
a & a & -a & -a \\
a & a & a & -a \\
a & -a & a & a
\end{pmatrix} \cong \begin{pmatrix}2a & -2a & 0 & -a \\
0 & 2a & -2a & a \\
2a & 0 & 2a & -a \\
0 & 0 & 0 & a
\end{pmatrix}
\]

For symmetry, the procedure described in the proof of Proposition \ref{prop:lempg} is repeated. \(\blacksquare\)

This second lifting relates the graphs obtained to the family of Lipschitz graphs and quaternion algebras, introduced in \cite{21}, for obtaining perfect codes over 4D spaces. This graph will be denoted as Lip(a).

Finally, there are several ways of lifting the BCC, although none of them preserves the symmetry as proved in the next theorem.

Theorem 20. Any lift of BCC yields a non-edge-symmetric graph.

Proof. Let \(M = \begin{pmatrix}2a & 0 & a \\
0 & 2a & a \\
0 & 0 & a\end{pmatrix}\), \(BCC(a) \simeq G(M)\). Assume that exists a symmetric lift \(G(L)\) of \(BCC(a)\).

\[
L = \begin{pmatrix}2a & 0 & a & x \\
0 & 2a & a & y \\
0 & 0 & a & z \\
0 & 0 & 0 & t\end{pmatrix}
\]

In Hermite form we have \(0 \leq x, y < 2a\) and \(0 \leq z < a\). For symmetry, the gcd of every row must be the same (map \(e_i\) into \(e_n\) and Gauss-reduce), hence \(t\) divides all the other entries of \(L\) and without loss of generality we assume \(t = 1\).

By \cite{8} we know that automorphisms are matrices \(P\) satisfying the condition that \(M^{-1}PM\) is an integer matrix where \(P\) is unitary and only has \(\pm 1\) entries. Both, the sets of these matrices which would give edge-transitivity, and the possible lifts, are finite. Hence we can run a computation which gives the negative result.

As we have concluded before, there is no decisive interest in obtaining a symmetric graph in 4D such that its 3D partitions remain themselves symmetric. Therefore, we could explore which of the lattice graphs whose projection is a BCC would be the most interesting.

Figure \ref{fig:liftings} summarizes how the previous constructions can be generalized to any number of dimensions. The procedure is represented in a tree. In this tree, nodes are the matrices of the lattice graphs. Note that, for an easier visualization, matrices have been normalized by dividing them by \(a\). Hence, each child is a lift of its parent. Moreover, we have restricted lifts to those whose side is greater or equal to the half of the side of its projection, otherwise many more graphs would appear.

The root of the tree is the matrix associated with a cycle. The lifts of the cycle conserving symmetry, and fulfilling the restrictions mentioned above, are the torus and the twisted torus introduced in Section \ref{sec:tori}. Then, as we have seen in Section \ref{sec:lifting} the cubic crystal lattice graphs are lifts of these two. The two branches show that only two families are obtained. The left branch consists of the infinite family of symmetric tori or \(n\)-dimensional PC\(\)'s; and each \(nD\)-PC has a \(nD\)-BCC sibling which is a leaf, without any further symmetric lift. The right branch is the family of the \(n\)-dimensional FCC\(\)'s; the \(nD\)-FCC always has the \((n+1)D\)-FCC as a symmetric lift. Moreover, there are some dimensions (4 and 6 in the figure) in which a different lift exists. Interestingly, two non right-equivalent matrices generate the same graph (denoted with \(\sim\)). The two branches in the tree are really different and, as we show next, they can be used to obtain new hybrid lattice graphs.

4.2 Hybrid Graphs: Common Lift of Crystal Graphs

In this subsection a different approach for embedding crystal graphs is considered. Given a number of crystal graphs, the idea is to generate a lattice graph which has them as its projections. Let us introduce this concept in the next definition.

Definition 21. The lattice graph \(G(M)\) is a common lift of \(G(M_1)\) and \(G(M_2)\) if both can be obtained as projections of \(G(M)\).

Remark 22. There are several ways of obtaining different common lifts of two given lattice graphs. A straightforward one is to consider the lattice graph \(G(M_1 \oplus M_2)\) generated by the direct sum of the matrices. As we state next, this option leads to the Cartesian product of the two given lattice graphs.

Lemma 23. \(G(M_1 \oplus M_2)\) is a common lift of \(G(M_1)\) and \(G(M_2)\) and \(G(M_1 \oplus M_2) \cong G(M_1) \times G(M_2)\), which denotes the Cartesian product of \(G(M_1)\) and \(G(M_2)\).

As we will see next, there exist other common lifts which obtain \(G(M_1)\) and \(G(M_2)\) as projections but generating a
Theorem 24. Given two lattice graphs $G(M_1)$ and $G(M_2)$, we consider the lattice graph $G(M_1 \boxplus M_2)$ which is obtained as follows: Let $M_1 \cong H_1$ and $M_2 \cong H_2$ with $H_1$ and $H_2$ in Hermite normal form. Let $C$ be the submatrix with the first common columns of $H_1$ and $H_2$. Then $H_1 = \begin{pmatrix} C & R_A \\ 0 & A \end{pmatrix}$ and $H_2 = \begin{pmatrix} C & R_B \\ 0 & B \end{pmatrix}$, where $A$ and $B$ are square matrices. Then
\[ M_1 \boxplus M_2 = \begin{pmatrix} C & R_A & R_B \\ 0 & A & 0 \\ 0 & 0 & B \end{pmatrix} \]

It is obtained that:

i) $G(M_1 \boxplus M_2)$ is a common lift of $G(M_1)$ and $G(M_2)$.

ii) $\max(\text{dim}(G(M_1))), \text{dim}(G(M_2))) \leq \text{dim}(G(M_1 \boxplus M_2)) \leq \text{dim}(G(M_1) + G(M_2)) = \text{dim}(G(C)) + \text{dim}(G(M_1) + G(M_2)) = \text{dim}(G(M_1 \boxplus M_2))$

Proof. The first item is obtained by construction. For the second one, consider $\max(\text{dim}(G(M_1))), \text{dim}(G(M_2))) \leq \text{dim}(G(M_1 \boxplus M_2)) = \text{dim}(G(M_1)) + \text{dim}(G(M_2)) - \text{dim}(G(C)) \leq \text{dim}(G(M_1)) + \text{dim}(G(M_2)) = \text{dim}(G(M_1 \boxplus M_2))$

Note that when the matrices $M_1$ and $M_2$ have no common columns, both $G(M_1 \boxplus M_2)$ and $G(M_1 \oplus M_2)$ coincide. Moreover, by construction, the operation $G(M_1 \boxplus M_2)$ provides a lift which minimizes its dimension. As shown in the next example, to handle graphs using $\boxplus$ that belong to the same branch of the tree in Figure 4 have some advantages in this sense.

Example 25. The first one is the hybrid graph obtained as a common lift of the $PC(2a)$ and $BCC(a)$. The calculation described in the Theorem 24 leads to the matrix:
\[
\begin{pmatrix}
2a & 0 & 0 \\
0 & 2a & 0 \\
0 & 0 & 2a
\end{pmatrix} \boxplus \begin{pmatrix}
2a & 0 & a \\
0 & 2a & a \\
0 & 0 & a
\end{pmatrix} = \begin{pmatrix}
2a & 0 & 0 & a \\
0 & 2a & 0 & a \\
0 & 0 & 2a & a
\end{pmatrix}
\]

which corresponds to a $4D$ lattice graph. On the other hand, if we make the common lift of $PC(2a)$ and $FCC(a)$:
\[
\begin{pmatrix}
2a & 0 & 0 \\
0 & 2a & 0 \\
0 & 0 & 2a
\end{pmatrix} \boxplus \begin{pmatrix}
2a & a & a \\
0 & 2a & a \\
0 & 0 & a
\end{pmatrix} = \begin{pmatrix}
2a & a & a & 0 & a \\
0 & 2a & 0 & a & a \\
0 & 0 & 2a & a & a \\
0 & 0 & 0 & a & a
\end{pmatrix}
\]

which generates a $5D$ lattice graph. In this case, the common lift has one extra dimension since the graphs considered belong to different branches of the tree. The same happens with the mix of $FCC(a)$ and $BCC(a)$, as shown next:
Finally, to end the section we present in Table 2 a selection of lattice graphs composed following the guidelines presented in this section. The table also includes their main topological characteristics. Depending on the focus some of them outperform the others.

5 Routing in Lattice Graphs

Most interconnection networks use routing tables but their size can compromise system scalability. In this section routing algorithms for lattice graphs are presented. In this way, algorithmic routing can be used to avoid the need of tables. If tables are to be used, the algorithms presented can be employed to fill the routing tables.

Our routing algorithm is based on the hierarchy induced by the projecting operation. Routing in a lattice graph can be done by routing in its projection and in the ring defined by its side. In a first subsection we state the node labelling adopted and present a hierarchical routing. In a second subsection, we solve the routing problem in cubic crystal graphs; this is a basic contribution since we are considering cubic crystal graphs as the basic building blocks of the networks proposed in this paper. Finally, complexity and implementation aspects are considered in the last subsection.

5.1 Hierarchical Routing

For solving the routing problem over lattice graphs we need first to state which labelling set will be applied. A labelling set is the set which contains the labels for the vertices of the graph. There are many choices for the labelling set. In 2D case, several approaches to the routing problem have been made in [17, 26, 9]. In those articles, several labellings such as the one given by the fundamental parallelogram of the lattice, the set of integers modulo \( N \) or the set of minimum norm residues have been considered. Anyhow, for labelling a lattice graph of dimension \( n \), a subset of \( \mathbb{Z}^n \) will be needed. In particular, we define it as follows.

**Definition 26.** Given a lattice graph \( G(M) \) of dimension \( n \) a labelling set of the graph is \( \mathcal{L} \subset \mathbb{Z}^n \) such that \( |\mathcal{L}| = |\det M| \) and for every pair \( l_1, l_2 \in \mathcal{L} \) we have \( l_1 \neq l_2 \) (mod \( M \)).

If \( v_s, v_d \in \mathcal{L} \), where \( v_s \) labels the source node and \( v_d \) labels the destination node, we will call any vector \( r \in \mathbb{Z}^n \) a routing record when

\[
v_d - v_s \equiv r \pmod{M}.
\]

With \( v_d - v_s \in \mathbb{Z}^n \) such that:

\[
v_d - v_s \in \mathcal{L} - \mathcal{L} = \{ x - y \mid x, y \in \mathcal{L} \}
\]

From a design perspective, it is convenient to label the graph nodes according to their positive coordinates. Hence, we will consider the labelling given by the Hermite normal form of the generating matrix. Therefore, let us assume that \( H \) is the Hermite normal form of \( M \) and

\[
\mathcal{L} = \{ x \in \mathbb{Z}^n \mid 0 \leq x_i < H_{i,i} \}.
\]

The differences set that will be the input for any of the considered routing algorithms will be:

\[
\mathcal{L} - \mathcal{L} = \{ x \mid -H_{i,i} < x_i < H_{i,i} \}.
\]

Each component of a routing record indicates the number of hops in the corresponding dimension and its sign, the direction of the hops. The length of a path associated with a routing record is given by its Minkowski norm:

\[
|r| = \sum_i |r_i|
\]

As minimal routing requires shortest paths, minimum norm routing records should be obtained. Hence, the routing problem over \( G(M) \) can be stated as follows:

**input:** \( v := v_d - v_s \in \mathcal{L} - \mathcal{L} \),

**output:** \( \text{argmin}_{r \in \mathcal{L} - \mathcal{L}} (|r|) \)

where \( \text{argmin} \) states for the element in the set \( \{ r \in \mathbb{Z}^n \mid r \equiv v \pmod{M} \} \) minimizing \( |r| \).

Our routing approach takes advantage of the hierarchical nature of lattice graphs. The idea is that routing in a lifted graph can be done by routing in its projection and in the cycle that joins the disjoint projections. Remember that the lattice graph \( G(M) \) with \( M \equiv \begin{pmatrix} B & e \\ 0 & a \end{pmatrix} \), has a disjoint copies of its projection \( G(B) \) embedded, which are connected by \( \frac{\det M}{\text{ord}(e_n)} \) parallel cycles. The cycles have length \( \text{ord}(e_n) \). The number of vertices belonging to a cycle which lie in the same copy of \( G(B) \) is \( \frac{\text{ord}(e_n)}{a} \). Hence, we can separately consider the elements of the routing record in the following way:

**Proposition 27.** Let \( M \equiv \begin{pmatrix} B & e \\ 0 & a \end{pmatrix} \). Then, if \( \mathcal{L}_M \) denotes the labelling set \( G(M) \) and \( \mathcal{L}_B \) denotes the labelling set of its projection \( G(B) \) we deduce that:

\[
\mathcal{L}_M = \left\{ \begin{pmatrix} x \\ y \end{pmatrix} \mid x \in \mathcal{L}_B, 0 \leq y < a \right\}
\]

**Example 28.** The labelling of the BCC\((a)\) is:

\[
\left\{ \begin{pmatrix} x \\ y \\ z \end{pmatrix} \mid 0 \leq x < 2a, 0 \leq y < 2a, 0 \leq z < a \right\}
\]

Note that it can be obtained from the labelling of the torus \( T(2a, 2a) \) by adding the last component \( z \) fulfilling \( 0 \leq z < a \).

Now, we can state the following main result:
which contains $y$ times be several routing records with the same weight. In this
Remark 30. In the last step of Algorithm 1 there can some-

If $FCC$ a 3D-torus graph. Hence, we provide routing algorithms for
minimum routing records in cubic crystal graphs. Routing in
We now consider specific algorithms for computing mini-

Table 2: Distance properties of several lattice graphs

| Topology         | Dimension | Order | Projection | Diameter | Average Distance |
|------------------|-----------|-------|------------|----------|------------------|
| $T(2a, 2a)$      | 3         | $4a^2$| vary       | $2a$     | $\approx 1.1487a$|
| 4D-FCC(a)        | 4         | $2a^4$| $FCC(a)$  | $2a$     | $\approx 1.1039a$|
| 4D-BCC(a)        | 4         | $8a^4$| $T(2a, 2a, 2a)$ | $2a$ | $\approx 1.5379a$|
| Lip(a)           | 4         | $16a^4$| $FCC(2a)$ | $3a$     | $\approx 1.815a$|
| PC(2a) $\circledast$ BCC(a) | 4         | $8a^4$| vary       | $2.5a$   | $\approx 1.5971a$|
| PC(2a) $\circledast$ FCC(a) | 5         | $8a^5$| vary       | $3.5a$   | $\approx 1.8785a$|
| BCC(a) $\circledast$ FCC(a) | 5         | $4a^5$| vary       | $2.5a$   | $\approx 1.5252a$|

Algorithm 1: Hierarchical Routing in Lattice Graphs

Input: $v_s$ source, $v_d$ destination
Output: $r$ minimum routing record from $v_s$ to $v_d$
Let $y$ be the last component of $v_d$;
$v_s + \mathcal{C}$ is the cycle translated to $v_s$;
For all the vertices $c_i$ of the cycle in the copy $[\mathcal{G}(B)]_y$
do:
$r_i^2$: Route in the cycle from $v_s$ to vertex $c_i$;
\[ r_i^G(B) \]: Route in $[\mathcal{G}(B)]_y$ from $c_i$ to $v_d$;
Return the routing record which minimizes the weight
of $r_i^G(B)$;

\[ r := \text{argmin}(|k| \mid k \in \{ r_1^G(B), r_2^G(B) \}) \];

Theorem 29. If $[\mathcal{G}(B)]_y$ is the projection $\mathcal{G}(B)$ of $\mathcal{G}(M)$
which contains $ye_n$, $\mathcal{C}$ denotes the cycle generated by $e_n$
and, given a vertex $v \in \mathbb{Z}^n$, $v + \mathcal{C}$ denotes the translation of
the cycle to this vertex. Algorithm 1 gives minimum routing
records in any lattice graph.

Proof. Since the algorithm composes routing records from
two subgraphs, then the result is indeed a routing record.
We need to see that a minimum one is found.
Let $r_{\text{min}}$ be one of the routing records with minimum
norm. Since $v_s + r_{\text{min}}$ is in the cycle mentioned in the algo-

remn, there is an index $i$ such that $r_{\text{min}}$ is the minimum
route in the cycle from $v_s$ to $c_i$. As $r_{\text{min}}$ is minimal, we find
that the minimal routing from $c_i$ to $v_d$ does not use the $n$
dimension. Thus, routing in $[\mathcal{G}(B)]_y$ gives the minimum.
By composing both, the algorithm finds the minimum routing
$r_{\text{min}}$ and returns it or another one with same norm. $\square$

Remark 30. In the last step of Algorithm 1 there can some-
times be several routing records with the same weight. In this
case it is advisable to choose one of them at random, thus
balancing the use of the paths.

5.2 Routing in Cubic Crystal Graphs

We now consider specific algorithms for computing mini-

\[ \begin{pmatrix} 2a & a & a \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix} \]
is isomorphic to the PDTT presented in [7], where a generic

These new algorithms are also based on the previous idea
of a hierarchical routing by using the projections of
the graphs. In general, we will denote a call to a routing algo-

\[ \text{Algorithm 2: Routing in FCC(a)} \]

Input: $(x, y, z)^T := v_d - v_s \in \mathcal{L} - \mathcal{L}$
Output: $r$ minimum routing record from $v_s$ to $v_d$
\[ y' := y + a(y < 0); \]
\[ z' := z + a(z < 0); \]
\[ x' := x + a((y < 0) \lor (z < 0)); \]
\[ x' := (y < 0) - 2a(x \geq 2a); \]
We have $(x', y', z') \in \mathcal{L}$;
\[ r_1^G(B) := \text{route}_{(2a \ a \ 0 \ a \ 0 \ 0)}((0 \ 0 \ y')); \]
\[ r_2^G(B) := \text{route}_{(2a \ a \ 0 \ a \ 0 \ 0)}((0 \ 0 \ y')); \]
\[ r := \text{argmin}(|k| \mid k \in \{ r_1^G(B), r_2^G(B) \}) \];

Remark 31. When $a$ is a power of 2 the starting arithmetic
operations are easier to calculate as \( \text{rem}(y,a) \), \( \text{rem}(z,a) \) and \( \text{rem}(\hat{x},2a) \).

**Algorithm 3:** Routing in \( \text{RTT}(a) \)

**Input:** \( x,y := v_d - v_s \)
**Output:** \( r \) routing record
\[
\begin{align*}
p & := \text{rem}(x + y + a,2a); \\
q & := \text{rem}(y - x + a,2a); \\
x' & := (p - q)/2; \\
y' & := (p + q - 2a)/2; \\
r & := (x',y');
\end{align*}
\]

**Example 32.** As an example let us consider FCC(4). The labeling of the graph is:
\[
\mathcal{L} = \{(x\ y\ z)^t : 0 \leq x < 8, \ 0 \leq y, z < 4\}.
\]
If we want to route from \( v_s = (1\ 3\ 3)^t \) to \( v_d = (6\ 0\ 1)^t \), first we compute \( v = v_d - v_s = (5\ -3\ -2)^t \), which is in the set of differences:
\[
v \in \mathcal{L} - \mathcal{L} = \{(x\ y\ z)^t : -8 < x < 8, -4 < y, z < 4\}.
\]
According to Algorithm 2, since we have \( y = -3 < 0 \) and \( z = -2 < 0 \) these values have to be modified as \( y' = -3 + 4 = 1 \) and \( z' = -2 + 4 = 2 \). Moreover, since \( (-3 < 0) \times (0 < 0) \equiv \text{false} \) we find that \( \hat{x} = 5 \). Finally, as \( 0 \leq 5 < 8 \) this implies \( x' = 5 \) and \( v \equiv (5\ 1\ 2)^t \in \mathcal{L} \).

Now, in \( \text{RTT}(a) \) we find that a minimum route from \( (0\ 0\ 0)^t \) to \( (5\ 1\ 1)^t \) is \( (1\ -3\ -2)^t \) and a minimum route from \( (4\ 0\ 0)^t \) to \( (5\ 1\ 1)^t \) is \( (1\ 1\ 1)^t \). Consequently, \( r_1 = (1\ -3\ -2)^t \) and \( r_2 = (1\ 1\ -2)^t \). Finally, after comparing the two norms \( |r_1| = 6 \) and \( |r_2| = 4 \), we find that the minimum routing record to reach \( v_d \) from \( v_s \) is given by \( r = r_2 \).

Similarly, for the network \( BCC(a) \), we obtain Algorithm 4. Again, the order \( \text{ord}(e_a) = 2a \) which implies 2 calls to the routing of a 2D torus \( T(2a,2a) \).

### 5.3 Routing Discussion

Routing in circulant graphs was first related to the Shortest Vector Problem (SVP) in [18]. Later, this fact was used to optimize a routing algorithm for circulants of degree four in [18]. Following the same ideas, similar complexity for the SVP can be inferred for routing in lattice graphs. However, algorithms for particular graphs can be improved. In this subsection we consider how to appropriately choose the projection of the lattice graph in order to obtain the best routing algorithm among all the possibilities.

First, note that following the ideas in the previous section, we can infer the impact of routing complexity for the different lifts of crystal lattice graphs. As we have seen, \( \text{ord}(e_a) \) determines the number of intersections of the cycle with the destination projection, which dictates the number of nested routing calls.

### 6 Practical Issues

This work has been conceived to study the fundamentals of twisting wrap-around links in multidimensional torus networks. Nevertheless, this research has been motivated by the...
widespread presence of moderate degree tori in the super-computing market. Although Fujitsu has recently entered in this terrain with its K system, traditionally Cray and IBM are the two major companies standing out for years in the development of interconnection networks based on torus networks. Hence, this section will be devoted to discuss certain practical aspects. The first one is related to physical network deployment and the second consists of a preliminary performance evaluation.

6.1 Physical Organization

It is not difficult to conceive a package hierarchy and a 3D physical organization to deploy systems based on lattice graphs. For illustrating this organization, let us first consider the approach followed by manufacturers. Cray uses a straightforward structure. For example, an actual configuration, [5], was a T(25, 32, 16) packaged on a 200 rack system arranged as an 8 × 25 rectangle. We can see the system as:

- System of 25 × 8 × 1 racks.
- Racks of 1 × 4 × 16 nodes.

That is, the third dimension is completely inside the racks and the first dimension is formed entirely joining racks. However the second dimension is partially inside the rack and requires connecting rack columns by rings. Taking into account forthcoming improvements in integration and packaging technologies, it could be expected that a 4D torus would have two dimensions internal to the racks and the other 2 external to the racks. This idea generalizes to lattice graphs. If G(M) is a 4D lattice graph, its 2D projections would be built inside racks, which would be a torus or a twisted torus. Then it becomes a matter of completing the lattice by adjusting the offsets of the cables connecting the racks. Moreover, folding techniques for 3D networks presented in [7] can also be of application in our case and easily generalized to higher dimensions.

IBM presents a more elaborated organization in the Blue Gene family, [13]. Although the complete network is a torus, each midplane (half of a rack) has additional hardware which enables the midplane to disconnect from the remainder of the network and to be itself a small torus. By arranging several midplanes, this additional hardware enables a multitude of different tori shapes to be connected. With slight modifications to such hardware it is possible to allow each group to be a symmetric crystal (or another lattice if desired) instead of a mixed-radix torus. This hardware changes its configuration only between different application runs. Then, the potentially added functionality would not have any negative impact on the system.

6.2 Evaluation compared to currently used topologies

Most evaluations of big networks have relied on measuring their behavior when managing synthetic traffic loads. Typical experiments are based on simulation. Notwithstanding, the work presented in [11] evaluates different routing algorithms reporting maximum achievable loads on a real IBM BlueGene system. They make runs on machines whose topologies are the torus T(8, 8, 4, 2) and T(16, 8, 8, 2). We shall ignore the last dimension of size 2 and treat them as four dimensional networks; the last small dimension comes from the inside of computing nodes, fixed by computer technology. We have simulated the same tori plus symmetric lattice graphs of the same sizes. We evaluate 4D-BCC(4) compared to T(8, 8, 4, 2) and 4D-FCC(8) compared to T(16, 8, 8, 2).

We have used the same synthetic traffic patterns as in [11]:

- **uniform**: Each node generates packets to any other node, at random with a uniform probability distribution.
- **antipodal**: Each node generates traffic to the most distant one.
- **centralsymmetric**: Once a center of symmetry is fixed, each node has as its destination the symmetric one.
- **randompairings**: The network is divided into pairs in a random uniform way, which then communicate for all the simulation.

Simulations have been conducted using INSEE (Interconnection Network Simulation and Evaluation Environment) [23]. Their basic units are the *cycle* for measuring time and the *phit* for measuring information. Each network link (edge of the graph) can send one or zero phits in each cycle. The network *load* is the amount of information received per time. We measure the network load in phits/(cycle · node). Nodes (vertices of the graph) generate packets composed of integral number of phits (typically constant) to be sent to other network nodes. For any provided traffic up to load l, a packet is injected each cycle in each node with probability l/s, where s is the size of a packet measured in phits. The accepted traffic or throughput is the total of phits received, divided by the total simulation time and by the number of nodes N. Simulation parameters are shown in Table 3. We have simulated 10,000 cycles for statistics,

| Injectors | 6 |
| Packet size | 16 phits |
| Queues | 4 packets |
| Deadlock avoidance | Bubble |
| Virtual Channels | 3 |
| flow control | Virtual Cut-through |
| Routing Mechanisms | DOR |
| Arbitration mechanism | random |

Table 3: Simulation parameters
preceded by a network warmup. At least 5 simulations are averaged for each point. The BlueGene family of supercomputers implements a congestion control mechanism that prioritizes in-transit traffic over new injections, which is also implemented in our router model.

Figures 5 and 6 show results of accepted load in the four networks. Under uniform traffic, results exhibit gains of 26% in the small case ($4D$-BCC(8)) and 50% in the large one ($4D$-FCC(8)). In random pairings, the throughput is consistently higher, with gains of 16% and 2% respectively. The other two traffic patterns show congestion at high loads for all the networks considered. Nevertheless, the peak load for the antipodal traffic improves by 62% and 75% respectively. Under central symmetric traffic, gains are of 45% in the small case and of 23% in the large one. Figures 7 and 8 show average packet latencies. The different curves demonstrate the superior behavior of lattice topologies. Gain values are coherent with the topological analysis presented in Subsection 3.4.

7 Conclusions

This research has been focused on the study and proposal of new multidimensional twisted torus interconnection networks. Due to their complex spatial characteristics, their analysis is far from straightforward. Nevertheless, we have taken advantage of an algebraic tool based on integral square matrices presented in [16]. Such matrices define the graph and its topological characteristics. Adequate algebraic manipulations of the matrices enable a better understanding of different network properties. For example, when using the Hermite normal form, matrices reveal the subgraphs naturally embedded in the network.

Using this tool, several networks have been proposed and analyzed in this paper. We firstly focus on 3D symmetric networks as alternatives to mixed-radix tori which are not edge-symmetric. Taking the matrices that define cubic crystallographic lattices, we were able to evaluate and compare their associated interconnection networks. If symmetry is desired, the best path when upgrading 3D systems clearly seems to be $PC(a) \rightarrow FCC(a) \rightarrow BCC(a) \rightarrow PC(2a)$, that is, duplicating the machine size on each step and maintaining most of the original connections. In addition, we have introduced a couple of graph lifting methods that allow for higher dimensional networks that embed cubic crystal sub-networks among other graphs. Complementarily, the use of graph projections facilitates the conception of routing algorithms for these networks. Based on this graph operation, minimal routing schemes have been proposed for all the topologies. Although we have focused on typical network configurations derived from powers of two, our results remain valid for any other network size.

The paper preliminarily addresses some practical issues. Physical packaging and system organization in racks have been considered, concluding that, for deploying networks based on lattice graphs, very few changes over typical tori would be necessary. In addition to the algebraic analysis carried out through the paper, an empirical evaluation of
different interesting topologies has been carried out. Comparisons with current machines have certified that multidimensional twisted tori clearly outperform their orthogonal counterparts. Noticeable gains were exhibited by twisted lattice topologies for both configurations under consideration. These preliminary experiments motivate a thorough network evaluation that will be reported in a forthcoming work.

A Symmetric Lattice Graphs of dimension 3

This Appendix provides a complete characterization of those lattice graphs which are edge-symmetric by linear automorphisms. In Subsection A.1, some definitions and preliminary lemmas are obtained. In Subsection A.2, the complete characterization is done. Finally, some additional comments on the non-linear case are done in Subsection A.3

A.1 About linear automorphisms

Definition 34. A signed permutation of length \( n \in \mathbb{N} \) is a composition of a sign changing function \( (k \rightarrow \pm k, 1 \leq k \leq n) \) and a permutation \( \pi \in \Sigma_n \).

Then, we call signed permutation matrix to a matrix such that when it multiplies a vector it applies the signed permutation to the vector. Signed permutation matrices are the matrices such that in each row and column all entries are zero except exactly one entry with value \( \pm 1 \).

In \([8]\) the two following results were proved.

Lemma 35. For any linear automorphism \( \phi \) of \( G(M) \) with \( \phi(0) = 0 \) there exists a signed permutation matrix \( P \) such that \( \phi(x) = Px \).

Lemma 36. The function \( \phi \) defined by \( \phi(x) = Px \) is an automorphism of \( G(M) \) if and only if there exists \( Q \in \mathbb{Z}^{n \times n} \) such that \( PM = MQ \).

The linear automorphisms of a lattice graph \( G(M) \) form a group \( LAut(G(M)) \), which usually coincides with the full automorphism group \( Aut(G(M)) \), except in a few cases that we consider in the last section of this appendix. The group of linear automorphisms which fixes 0 will be denoted as \( LAut(G(M), 0) \) (also known as stabilizer).

Definition 37. We say that \( G(M) \) is linearly-symmetric if for every \( i \) there exist \( \phi \in LAut(G(M), 0) \) such that \( \phi(e_i) = \pm e_i \).

Lemma 38. A linearly-symmetric lattice graph is symmetric.

We can denote signed permutations as \((1 -2)(-3 -4), \) where \( \sigma = (\ldots \pm a b \ldots) \) means that \( \sigma(a) = b = -\sigma(-a) \) and \( \sigma = (\ldots \pm a -b \ldots) \) means that \( \sigma(a) = -b = -\sigma(-a) \). The number of signed permutations of length \( n \) is \( n!2^n \). For \( n = 3 \) this is \( 3!2^3 = 48 \), which are shown in Table [11]

A.2 Determination of all linearly symmetric lattice graphs for \( n = 3 \)

Definition 39. A pair of matrices \( A, B \in \mathbb{Z}^{n \times n} \) are similar when a unit matrix \( U \) exists such that \( AU = UB \). This is denoted by \( A \sim B \).

Lemma 40. Let \( PM = MQ \) and \( PM' = M'Q' \) then \( M \cong M' \iff Q \sim Q' \).

Proof. We see that if we know \( PM = MQ \) and \( M = M'U \) then \( PM'U = M'UQ \) and \( PM' = M'(UQ^{-1}) = M'Q' \) with \( Q' \sim Q \). Reciprocally, we know that if \( PM = MQ \) and \( Q' = UQ^{-1} \) then \( M' = MU \) produces \( PM' = M'Q' \) and \( M' \cong M \).

Since right equivalences leave the group invariant (hence the graph is the same), we know that for a given \( P \) we only need to see how many \( Q \) there are modulo similarity. Then, knowing \( P \) and \( Q \) we can solve for \( M \).

In \([23]\) the following useful theorem is stated:

Theorem 41. Given a matrix \( A \) we can find a similar matrix, made of blocks, which is block upper triangular and moreover, that the blocks of the diagonal all have characteristic polynomial irreducible over \( \mathbb{Q} \) (Theorem III.12, page 50).

One simple case is when \( LAut(G(M), 0) \) is a cyclic group \( \langle \phi \rangle \). In this case the associated matrix will have characteristic polynomial \( x^n \pm 1 \). Starting at \( n = 4 \) we can find groups, such as the Klein four-group in which the group is generated by more than 1 element.
Lemma 42. Given $M \in \mathbb{Z}^{3 \times 3}$, $G(M)$ is linearly symmetric if and only if there exists a signed permutation of order 3 in $LAut(G(M), 0)$.

Proof. If such a signed permutation exists, it is clear that $G(M)$ is linearly symmetric.

For the reciprocal, we begin noting that signed permutations of length 3 can have orders 1, 2, 3, 4 and 6. The identity is the only signed permutation of order 1 and does not contribute to symmetry. Moreover, the signed permutations which only change signs (such as $(-1)(2)(-3)$) do not contribute to symmetry. Any remaining signed permutation of orders 2 and 4 do not provide symmetry by themselves, and the composition of two of them generates either a sign change or a permutation of order 3 or 6.

Hence linear symmetry implies the existence of an automorphism $\phi \in LAut(G(M, 0))$ with order 3 or 6. If it has order 3, we already have the desired permutation. Otherwise we have $\phi^3 = -id$ and so $\psi = \phi^2$ has order 3.

Hence, if $G(M)$ is linearly symmetric then $LAut(G(M), 0)$ contains at least one of the next four groups as a subgroup and there is a matrix $P$ such that $PM = MQ$ for some $Q$.

- $\langle (1 2 3) \rangle = \langle (1 3 2) \rangle$ with $P_1$.
- $\langle (1 -2 -3) \rangle = \langle (-1 3 -2) \rangle$ with $P_2$.
- $\langle (-1 2 -3) \rangle = \langle (1 -3 -2) \rangle$ with $P_3$.
- $\langle (-1 -2 3) \rangle = \langle (-1 -3 2) \rangle$ with $P_4$.

$$
\begin{align*}
P_1 &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, & 
P_2 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \\
P_3 &= \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, & 
P_4 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \end{pmatrix}.
\end{align*}$$

These signed permutations have characteristic and minimum polynomial $x^3 - 1$. We can find some matrices (symbolic over 3 integer parameters) by taking $Q = P$, that is, we obtain $M_1$ such that $P_1 M_1 = M_1 P_1$. They are:

$$
\begin{align*}
M_1 &= \begin{pmatrix} a & c & b \\ b & a & c \\ c & b & a \end{pmatrix}, \\
M_2 &= \begin{pmatrix} a & -c & -b \\ b & a & -c \\ c & b & a \end{pmatrix}, \\
M_3 &= \begin{pmatrix} a & -c & -b \\ b & a & c \\ c & b & a \end{pmatrix}, & 
M_4 &= \begin{pmatrix} a & c & b \\ b & a & c \\ c & b & a \end{pmatrix}.
\end{align*}$$

We now need to find the similar matrices.

Lemma 43. There are exactly 2 similarity classes with characteristic polynomial $x^3 - 1$:

$$
\begin{align*}
Q_1 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}, & 
Q_2 &= \begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}.
\end{align*}$$
Proof. For $x^3 - 1 = (x-1)(x(x+1)+1)$ we have the following upper triangular block matrix which has its characteristic polynomial: $Q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}$. We know that

$$
\begin{bmatrix}
1 & m+2n & m-n \\
0 & -1 & 1 \\
0 & -1 & 0
\end{bmatrix}
= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}
$$

So $\begin{pmatrix} 1 & m+2n & m-n \\
0 & -1 & 1 \\
0 & -1 & 0 \end{pmatrix} \sim \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}$. And as $\det(\begin{pmatrix} -1 & -2 \\ 0 & 1 \end{pmatrix}) = 3$, by Theorem [11] we have at most 3 matrices modulo similarity, which are:

$$
\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 2 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}.
$$

We check that the first two are non-similar. If

$$
\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}
= \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix}
\Rightarrow
\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix}
= \begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}
$$

Then

$$
\begin{pmatrix} a & b & c \\ -d-g & -e+h & -f+i \\ -d & -e & -f \end{pmatrix}
= \begin{pmatrix} a & b & c \\ -d-b-c & a+b \\ d+e & e+f & -d \end{pmatrix}
$$

Hence $d = g = 0$ and $a = -3b$, and $3b$ divides the determinant, which cannot be a unit. Now we see that the last two are similar.

$$
\begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}
= \begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}
$$

So we have proved that there are exactly 2 similarity classes with characteristic polynomial $x^3 - 1$:

$$
Q_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix} \text{ and } Q_2 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{pmatrix}.
$$

And now that $P_1 \sim P_2 \sim P_3 \sim P_4$.

$$
\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}
= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\Rightarrow
\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}
= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
$$

Thus, the first 4 matrices with $P_iM = MQ_i$ are right equivalent to the previously calculated $M_i$.

Now we find the 4 symbolic matrices $M'_i$ which satisfy $P_iM'_i = M'_iQ_1$.

$$
M'_1 = \begin{pmatrix} a & b & c \\ a & c & -b-c \\ -a & -b-c & b \end{pmatrix}
M'_2 = \begin{pmatrix} a & b & c \\ -a & -c & b+c \\ a & -b-c & b \end{pmatrix}
M'_3 = \begin{pmatrix} a & b & c \\ -a & b+c & -b \\ a & -c & b+c \end{pmatrix}
M'_4 = \begin{pmatrix} a & b & c \\ -a & -c & b+c \\ a & b+c & -b \end{pmatrix}
$$

Thus the next two lemmas show that the 8 families of matrices modulo similarity are actually only 2 families modulo graph isomorphism.

**Lemma 45.** The sets induced by the matrices $M_1$, $M_2$, $M_3$ and $M_4$ are the same modulo graph-isomorphism when taking the parameters $a, b, c \in \mathbb{Z}$.

**Proof.**

$$
\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
M_1 \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
= \begin{pmatrix} -a & c & b \\ b & -a & c \\ c & -b & -a \end{pmatrix}
$$

which is $M_4$ giving $a$ the value $-a$.

$$
\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
M_1 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
= \begin{pmatrix} -a & c & -b \\ b & -a & c \\ -c & b & -a \end{pmatrix}
$$

which is $M_2$ giving $a$ the value $-a$ and $c$ the value $-c$.

$$
\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
M_1 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
= \begin{pmatrix} a & c & -b \\ b & a & c \\ -c & b & a \end{pmatrix}
$$

which is $M_3$ giving $c$ the value $-c$. 

\[\square\]
Lemma 46. The sets induced by the matrices $M'_1$, $M'_2$, $M'_3$ and $M'_4$ are the same modulo graph-isomorphism when taking the parameters $a, b, c \in \mathbb{Z}$.

Proof.

\[
M'_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad M'_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad M'_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad M'_4 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

Theorem 47. Any linearly symmetric lattice graph of dimension 3 is isomorphic to another generated by one of the matrices

\[
M_1 = \begin{pmatrix} a & c & b \\ b & a & c \\ c & b & a \end{pmatrix} \quad \text{or} \quad M'_1 = \begin{pmatrix} a & b & c \\ a & c & -b-c \\ a & -b-c & b \end{pmatrix}
\]

for some $a, b, c \in \mathbb{Z}$.

Proof. Let a linearly symmetric lattice graph $G(M)$ with $M \in \mathbb{Z}^{3 \times 3}$. By Lemma 42, $P$ must exist with $PM = MQ$ with $P \in \{P_1, P_2, P_3, P_4\}$. By Lemmas 40 and 43 there exist $M'$ and $Q$ with $M \cong M'$, $Q \in \{Q_1, Q_2\}$ and $PM' = M'Q$. If $Q = Q_2$, then by Lemma 44 we know $M'' \in \{M_1, M_2, M_3, M_4\}$ with $PM'' = M''P$, $M'' \cong M$, by Lemma 45 it follows that $G(M) \cong G(M'_1)$. If $Q = Q_1$, then by Lemma 44 we know $M' \in \{M'_1, M'_2, M'_3, M'_4\}$, thus by Lemma 46 we obtain that $G(M) \cong G(M'_1)$.

\[\square\]

A.3 Non-linear automorphisms

In some cases, there are no linear automorphisms which give symmetry, although some non-linear automorphisms do so. The following theorem first stated in [3] analyzes those cases.

Definition 48. We say that $a, b, c, d \in \pm \mathbb{B}_n$ form a 4-cycle in $G(M)$ if 0 = $a + b + c + d$. Then, we say that $G(M)$ has no nontrivial 4-cycles if $a, b, c, d \in \pm \mathbb{B}_n$ such that 0 = $a + b + c + d$ which implies $a = -b$ or $a = -c$ or $a = -d$.

Theorem 49. If the connected lattice graph $G(M)$ has no nontrivial 4-cycles then any graph automorphism with $\phi(0) = 0$ is a group automorphism of $\mathbb{Z}^n/\mathbb{M}\mathbb{Z}^n$.

For $n = 2$ all symmetric lattice graphs which are not linearly symmetric were determined, which are:

- The ones which had two linearly independent nontrivial 4-cycles.
- The ones with exactly one nontrivial 4-cycle.

\[\text{each of } \{(v, v + a, v + a + b, v + a + b + c, v + a + b + c + d) : v \in G(M) \} \text{ is a cycle of length } 4\]

The first item directly produces the matrices (plus their divisors), since they are combinations of $(4, 0), (3, 1), (2, 2)$ with the appropriate changes. For the second item, it was seen that the only ones were the family $\begin{pmatrix} m & 2 \\ n & 2 \end{pmatrix}$, which are the only ones which fail Adam-isomorphy [28].

For more dimensions, first we note all the possible non-trivial 4-cycles (up to adding zeroes and sign permuting):

- $(4, 1)$ first appearing at dimension $n = 1$
- $(3, 1)$, $(2, 2)$ first appearing at $n = 2$
- $(2, 1, 1)$ first appearing at $n = 3$
- $(1, 1, 1, 1)$ first appearing at $n = 4$

Symmetric graphs which are not linearly symmetric lattice graphs can be obtained by using one of the 4-cycles as a column, completing the matrix and checking if the matrix or one of its divisors generates a symmetric lattice graph. Here we will not perform the complete characterization of the symmetric lattice graph of dimension 3 having nonlinear automorphisms, since it does not contribute any insight to the discussion in the main paper.

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