Java-based Program for Computing the Wiener Index of a Body - Centered Cubic Graph*

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Abstract:

In chemical graph theory, Wiener index is a topological index of a molecule. The Wiener index of a graph G is equal to the sum of distances between all pairs of distinct vertices of G. It has been one of main descriptors that correlate a chemical compound's molecular graph with experimentally gathered data regarding the compound's characteristics. In this paper we calculate the Wiener index for body-centered cubic grid connected in a line. A Java-based program is designed to automatically compute the distances between centers, centers and border vertices, border vertices and the sum of all distances (Wiener index) for such grid.

Keywords: Wiener Index, Body-centered cubic grid, Face-centered cubic, Diamond grid, Shortest paths, Non-traditional grids.

ملخص بالعربية:

هدفت هذه الورقة العلمية الى ايجاد و حساب مؤشر وينر Wiener Index في نظرية الرسم البياني الكيميائي Chemical graph، مؤشر وينر هو مؤشر طوبولوجي مهم لتحديد بعض الصفات للعناصر. مؤشر وينر للرسم البياني G يساوي مجموع المسافات بين جميع الرؤوس داخل الرسم البياني الكيميائي. في هذه الورقة تم ايجاد برنامج يعتمد على لغة البرمجة جافا لحساب مؤشر وينر لمكعب مركزي الجسم (bcc) ذرة تشغل المركز. يقوم البرنامج بحساب اقصر المسافات بين جميع الرؤوس في الشكل الذي تم اعتماده في هذ الورقة العلمية وايجاد مجموع اقصر المسافات التي تربط هذه الرؤوس ومن ثم حساب مؤشر وينر لهذه الشبكة.

الكلمات المفتاحية: مؤشر وينر، شبكة مكعبة، مكعب مركزي الجسم، مكعب مركزي الوجه، أقصر المسافات، شبكات غير تقليدية.

INTRODUCTION

In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications (Alipour & Ashrafi, 2009). In recent research in mathematical chemistry, particular attention has been paid to so called topological indices. These are invariants which can be calculated from the underlying molecular graphs and hopefully exhibit good correlations with physical and chemical properties of the corresponding molecules (Mohar & Pisanski, 1988).

In this paper, unit cells are considered, for an example see Fig. 1. All graphs that are considered here are finite, undirected and simple. Throughout this paper we consider simple connected graphs, i.e. connected graphs without loops and multiple edges. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. If u and v are two vertices of G then dG(u,v) denotes the length of a minimal path connecting u and v (Alipour & Ashrafi, 2009a).

After having some preliminaries including an introduction to the chemical graphs, Body-Centered Cubic (bcc) Grid, and Wiener Index, an equations (lemmas) to compute the distances between centers, centers and border vertices, border vertices and the sum of all distances (Wiener index) for a body-centered cubic grid connected in a line are presented. A Java-based program to automatically compute these distances for such grid are also provided. Concluding remarks and further thoughts close the paper.

Chemical Graph

In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. Having a molecule, if we represent atoms by vertices and bonds by edges, we obtain a molecular graph. A chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds (Yamuna, 2014). In the framework of Bond-Valence theory, chemical graph theory views the

molecular structures of organic compounds, often referred to as molecular graphs in which atoms are represented by vertices and the covalent chemical bonds by edges.

Chemical Graph theory is used to model physical properties of molecules called alkanes. Indices based on the graphical structure of the alkanes are defined and used to model both the boiling point and melting point of the molecules (Baskar & Senbagamalar, 2012)

We first describe some notations which will be kept throughout the paper. A topological index of a graph G is a numeric quantity related to G .The oldest topological index is the Wiener index which introduced by Harold Wiener (Alipour & Ashrafi, 2009b). In chemical graph theory, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. Moreover, a chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Its vertices are labeled with the kinds of the corresponding atoms and the edges are labeled with the types of bonds (Thilakam & Sumathi, 2013).

Body-Centered Cubic (bcc) Grid

The body-centered cubic unit cell is the simplest repeating unit in a body-centered cubic structure. In bcc there are eight identical particles on the eight corners of the unit cell. A bcc unit cell has atoms at each corner of the cube and an atom at the center of the structure as we can see in Fig.1. According to this structure, the atom at the body center completely belongs to the unit cell in which it is present. The smallest repeating series of atoms in a crystal is called a unit cell. A third common packing arrangement in metals, the body-centered cubic (bcc) unit cell has atoms at each of the eight corners of a cube and one more atom in the center of the cube, because each of the corner atoms represents the corner of neighbored cube, the corner atoms in each unit cell will be shared among eight unit cells. The bcc unit cell consists of a net total of two atoms, the one in the center and eight at the corners.

The bcc unit cell is a cube (all sides are of the same length and all faces sharing a corner, making them perpendicular to each other) with an atom at each corner of the unit cell and an atom in the center of the unit cell (Kittel, 2004), (Strand & Nagy, 2007), and (Strand & Nagy, 2009). Each of the corner atoms is the corner of another cube. Thus, the corner atoms are shared among eight unit cells. It is said that bcc has a coordination number of 8 and a bcc unit cell consists of a net total of two atoms; one in the center and eight eighths from corner atoms. Some of the materials that have a bcc structure include potassium, chromium, barium, vanadium, alpha-iron and tungsten. When the metal is deformed, the planes of atoms must slip over each other, and this is more difficult in the bcc structure (Kittle, 2004). In Fig. 1 a bcc unit cell is shown, it is demonstrated that the closest atoms are connected to each other. Cesium chloride and some other salts also use the same structure in their crystals; having one type of atoms in the corners of a unit cell, and the other type in the center.

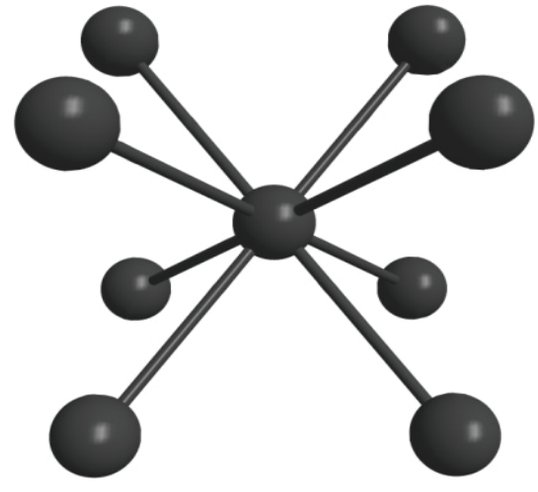


Fig. 1.

A unit cell of body-centered cubic (BCC) grid showing the neighbor relation of the atoms.

In this paper, we will compute wiener index for bcc connected in a line. Figure 2 below shows an example of such graph.

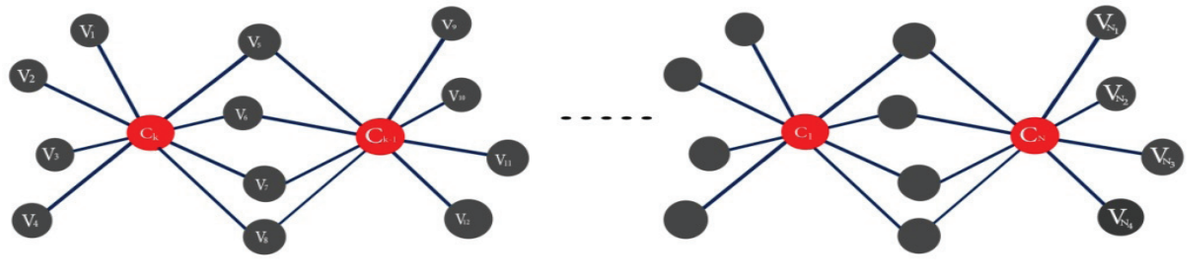


Fig.2.

k bcc unit cells connected in a row with a new unit cell attached at the end of the row.

Wiener Index

Topological indices have been defined as those "Numerical values associated with chemical contribution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity" (Baskar & Senbagamalar, 2012). The Wiener index is a graph invariant that belongs to the molecules structure-descriptors called topological indices, which are used for the design of molecules with desired properties (Randi ´c, 1993). At first, Wiener index was used for predicting the boiling points of paraffin's (Wiener, 1947), but later strong correlation between Wiener index and the chemical properties of a compound was found. Hence, Wiener index was used by chemists decades before it attracted the attention of mathematicians. In fact, it was studied long time before the development of the branch of discrete mathematics, which is now known as Graph Theory.

In (Wiener, 1947) Wiener introduced the notion of, as he called, path number of a graph. Actually, it was the sum of distances between any two carbon atoms in the molecules in terms of carbon-carbon covalent bonds. Subsequently, the index named after Wiener, is generalized to any graph G as:

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u,v) \qquad (1)$$

The sum of shortest distances for each pair of vertices of the graph G: the sum runs over all ordered pairs of vertices, and dG(u,v) denote the length of a shortest path in G between vertices u and v.

Definition: Let G be a graph with vertex set V(G) and edges aset E(G). The distance dG(u,v) between two vertices u,v∈ V(G) is the minimum number of edges on apth in G between u and v.

Wiener Index for a Row of bcc Unit Cells

In order to state the main formula that calculates the Wiener index for body-centered cubic grid connected in a line, first we have to state the following lemmas.

Sum of Distances between Center Points

Lemma 1. Let n bcc unit cells be connected in a row. Then the sum of all distances between center vertices in this bcc grid graph is given by:

$$\frac{n^3 - n}{3} \qquad (2)$$

The proof of Lemma 1 and the following Lemmas are given in Mujahed & Nagy, 2015.

Sum of Distances between Centers and Border Vertices

Lemma 2. (for proof see (Mujahed & Nagy,

2015)) Let n bcc unit cells be connected in a row. Then the sum of all distances between center vertices and border vertices in this bcc grid graph is given by

$$\frac{8n^3+12n^2+4n}{3} \quad (3)$$

Sum of Distances of Border Vertices

Lemma 3: (for the proof see (Mujahed & Nagy, 2015)). Let n bcc unit cells be connected in a row. Then the sum of all distances between pairs of border vertices is given by

$$\frac{16n^3+48n^2+68n+36}{3} \quad (4)$$

Sum of All Distances: The Main Formula

Based on the results proven in the previous three subsections, we are able to state our main result.

Theorem 1. (for the proof see (Mujahed & Nagy, 2015)) Let n be the number of bcc unit cells that are connected in a row. Then the formula to find WI for this graph is:

$$WI(n)=\frac{25n^3+60n^2+71n+36}{3} \quad (5)$$

Table 1 shows some of the first elements of the sequences we are working with, i.e., the values computed by equations (2), (3), (4) and (5) for some small values of n. The WI values are shown in the last row of the table.

Table 1.

Some values of the subsums and WI for few bcc cells in a row.

Number of bcc unit cells (n)	1	2	3	4	5	6	7	8	9	10
Equation (2)	0	2	8	20	40	70	112	168	240	330
Equation (3)	8	40	112	240	440	728	1120	1632	2280	3080
Equation (4)	56	164	368	700	1192	1876	2784	3948	5400	7172
Wiener Index WI	64	206	488	960	1672	2674	4016	5748	7920	10582

As we can see in table 1 above, the WI for single bcc is 64 (see figure 1). This means that the sum of total distance between all vertices (border vertices and center vertices) in this graph is 64. Now, according to figure 2, if we connect more bcc in the line, the sum of the total distance will be 206 for two connected bcc in a line (i.e. n=2).

A Java-Based Program for Computing the Wiener Index of Body-Centered Cubic Grid

Java is, arguably, one of the most popular programming languages among developers and it is used to create web applications, customized software and web portals, including e-Commerce and m-Commerce solutions (Georgiou, 2014). For many developers, programming languages begin and end with Java. Java programming language has many features that include fast platform independent (Williams, 2001).

Platform independent means java can run on any computer irrespective to the hardware and software dependency, and Java is fast because of Just In Time compiler (JIT) compiler. JIT compiler stores the repeated code in its cache memory and in byte code where repeated code is used , instead of loading that code again from memory, JIT use it from its cache memory which saves time and memory, and make execution fast.

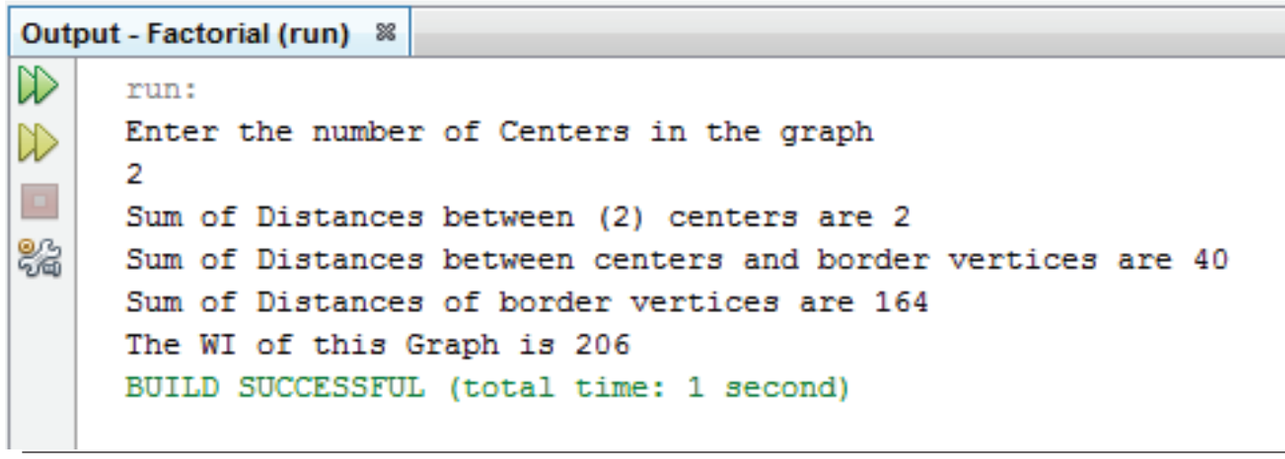
The following program (Program 3.1.1) illustrates the Wiener index for n body-centered cubic grid connected in a line.

Program: 3.1.1

```
package Wiener;
import java.util.Scanner;
public class Wiener {
static int factorial(int n){
 if (n == 0)
  return 1;
 else
  return(n * factorial(n-1));
}
 public static void main(String args[])
 {
   int n, centersums=0, vcsum=0, vvsum=0, WI=0;
    System.out.println("Enter the number of Centers in the graph");
    Scanner in = new Scanner(System.in);
    n = in.nextInt();
    if ( n <= 0 )
      System.out.println("Number of centers should be greater than zero.");
    else
    {centersums= (((n*n*n)-n)/3);
     vcsum= 2*(2*n+2)*(2*n+1)*(2*n)/(6);
vvsum=(16*(n+1)*(n+1)*(n+1)+20*(n+1))/(3);
      WI= (centersums+vcsum+vvsum);
       System.out.println("Sum of Distances between ("+n+") centers are "+centersums);
       System.out.println("Sum of Distances between centers and border vertices are
        "+vcsum);
      System.out.println("Sum of Distances of border vertices are "+vvsum);
      System.out.println("The WI of this Graph is "+WI);
       }
      }
    }
```

As it is shown in the program, first it asks the user to provide the number of the centers in the given graph. Then it calculates the sum of all distances between center vertices, the sum of all distances between center vertices and border vertices, and the sum of all distances between pairs of border vertices for this bcc grid graph. Then it calculates the WI by summing the values of these distances, and prints out the results.

Figure 3 below represents two examples that show the output of running the program to calculate the distances and the Wiener index for 2 and 10 body-centered cubic grids connected in a line. Using this algorithm helps in calculating the required distances in a way faster than doing this manually, specially for a grid that has a large number of bcc unit cells (n).



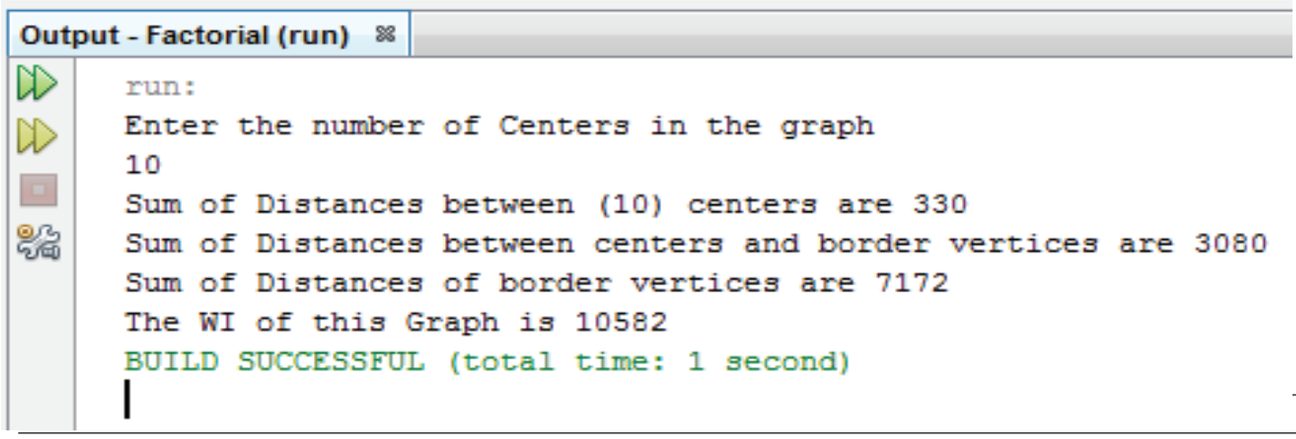


Fig.3.

The output of the designed program while running t to calculate the Wiener index for 2 and 10 body-centered cubic grid, connected in a line.

The same values that are shown in Table 1 are also obtaind when running the designed program for different bcc unit cells (n= 1 to 10).

CONCLUSION

The wiener index is one of the oldest molecular-graph-based structure-descriptors, and it is one of the current areas of research in mathematical chemistry. In (Harishchandra, Deepak, & Asha, 2012) the authors obtained the WI of line graphs and some other classes of graphs. In (Thilakam & Sumathi, 2014) a program for calculating the Wiener index of some Cycle related graphs is provided. The authors in (Daneshvar, Izbirak & Kaleibar, 2012) give explicit formula for WI of hypercubes and their corresponding Euclidean graph. In this paper, we have provided a new technique to compute topological indices for a specific type of graphs called body-centered cubic. One of the first, and most important, topological/geometrical indices of graph structure is the Wiener index. In this paper, the body-centered cubic grid is investigated in which a finite number of unit cells are placed next to each other at a line. A Java-based program is given to calculate the value of the Wiener index of such grids in a faster way. There are several ways to continue the line of the research that we have just started here such as:

- One can use programming language to compute Wiener index for other graph, e.g., Face-centered cubic and diamond grid and other non-traditional grids.
- One can extend the results to two and three dimensional rectangles and blocks of bcc unit cells.
- Weiner index is just one of many types of indices in molecular graphs. So we suggest to calculate other types of indices (i.e. Zagreb indices, edge Wiener, …etc.) and compare the new results with our results in this paper.

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