Discrete Optimal Global Convergence of an Evolutionary Algorithm for Clusters under the Potential of Lennard Jones

Carlos Barrón-Romero
cbarron@correo.azc.uam.mx

Universidad Autónoma Metropolitana, Unidad Azcapotzalco
Av. San Pablo No. 180, Col. Reynosa Tamaulipas, C.P. 02200,
MEXICO

2016

Abstract

A review of the properties that bond the particles under Lennard Jones Potential allow to states properties and conditions for building evolutive algorithms using the CB lattice with other different lattices. The new lattice is called CB lattice and it is based on small cubes, such the number of its vertices in a region is always greater than the number of the particles of a cluster or a region of a lattice inside of the same size region of the CB lattice. Moreover, the estimation of a putative optimal cluster of the Lennard Jones can be done theoretically in short time but, the proof, for such cluster to be the global optimal cannot be determining in efficient time. The proof of the global optimality for a cluster is related to the binomial coefficient $\binom{m}{n}$, which it corresponds with the selection of n particles from a collection with m given particles. A set of propositions states convergence and optimal conditions over the CB lattice for an evolutionary algorithm. The evolutionary algorithm is a reload version of previous genetic algorithms based in phenotypes. The novelty using CB lattice, together with the other lattices, and ad-hoc cluster segmentation and enumeration, is to allow the combination of genotype (DNA coding for cluster using their particle's number) and phenotype (geometrical shapes using particle's coordinates in 3D). A parallel version of an evolutionary algorithm for determining the global optimality is depicted. The algorithm for determining global optimality (which it is far from this research, and it is not included) is just a force brute searching algorithm with complexity $\binom{m}{n}$, where n is the number of the cluster's particles and $m \gg n$ is the number of particles of an appropriate CB lattice's region. The results presented are from a standalone program for a personal computer of the evolutionary algorithm, which can estimate all putative Optimal Lennard Jones Clusters from 13 to 1612 particles. The novelty are the theoretical results for the evolutionary algorithm's efficiency, the strategies with phenotype or genotype, and the classification of the clusters based in an ad-hoc geometric algorithm for segmenting a cluster into its nucleus and layers. Also, the standalone program is not only capable to replicate the optimal Lennard Jones clusters in The Cambridge Cluster Database (CCD), but to find new ones.

Keywords: 02.60.Pn Numerical optimization, 21.60.Gx Cluster models, 31.15.Qg Molecular dynamics and other numerical methods, 36.40.Qv Stability and fragmentation of clusters, Lennard Jones Potential.

1 Introduction

The problem for determining optimal clusters under Lennard Jones captures my attention for the possible implications for building an efficient algorithm for the class of NP. My techniques for the NP Class has an application for building an appropriate algorithms for looking the optimal clusters under Lennard Jones Potential.

Over a decade ago, I states the conjecture in [2] that IF lattice could contain all optimal clusters under the Potential of Lennard Jones (LJ). The title of the article: Minimum search space and efficient methods for structural cluster optimization was proposed as result of some inquiries from D. J. Wales, J. P. K. Doye, G.L. Xue and Bern Hardke about the optimal LJ clusters.

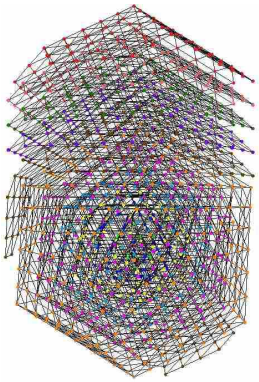
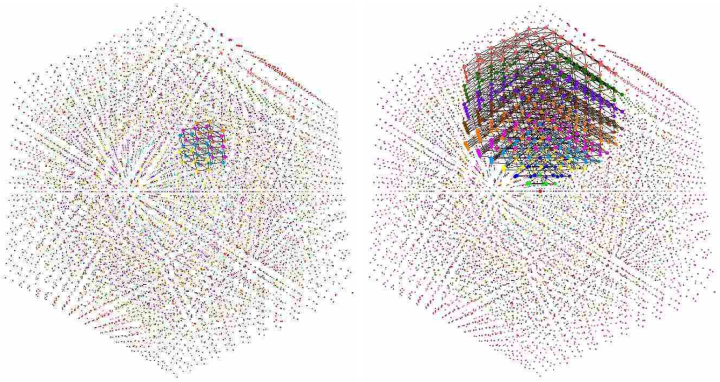


Figure 1: MIF1739 contains the initial particles' positions for the C_n^*, $n = 2, \ldots, 1000$.



a) b)

Figure 2: a) C_{38}^* and b) C_{664}^* inside of a region of the IF lattice.

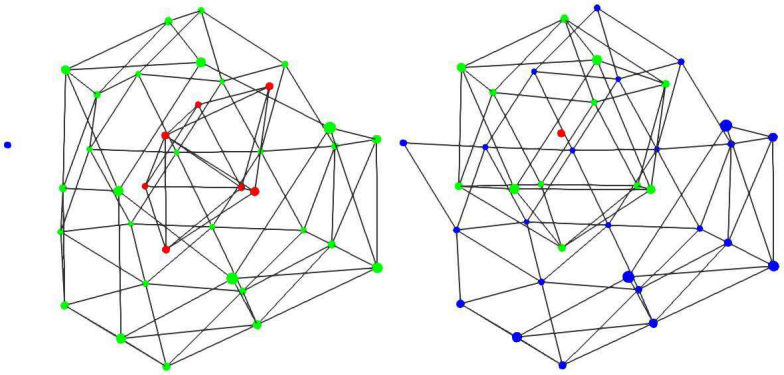
IF lattice results from overlapping the positions of the IC lattice and FC lattice. The main result was a minimum region of IF, where all putative global optimal LJ clusters from 2 to 1000 can be found (see figures 1, and 2).

Figure 1 was constructed by the selection of not repeated positions from where a given initial selection of particles converges always by a local minimization process to its putative minimal LJ cluster. This set of positions is finite, and it can be enumerate, such each position corresponds with a unique id number.

Therefore, it could be simple to locate a minimal LJ cluster by the set of its particles' number of the cluster. I proposed a telephone algorithm, which is like make a phone call but, here n id particles corresponds to a cluster's phone number from a set of an appropriate selection of m id numbers from a region of IF lattice. After the minimization if the value of the LJ potential is less than a previous cluster's number, then it is the phone number of the cluster of n particles. Even, it is like more genotype, I did not introduce this type of DNA mechanics in my previous genetic and evolutive algorithms in order to keep a phenotype representation (this means geometric shapes using the 3d particles' coordinate). The main idea was to look for the putative optimal LJ cluster by an exhaustive searching. This is a brute force algorithm with complexity related to the Newton binomio for combinations, $\binom{m}{n}$.

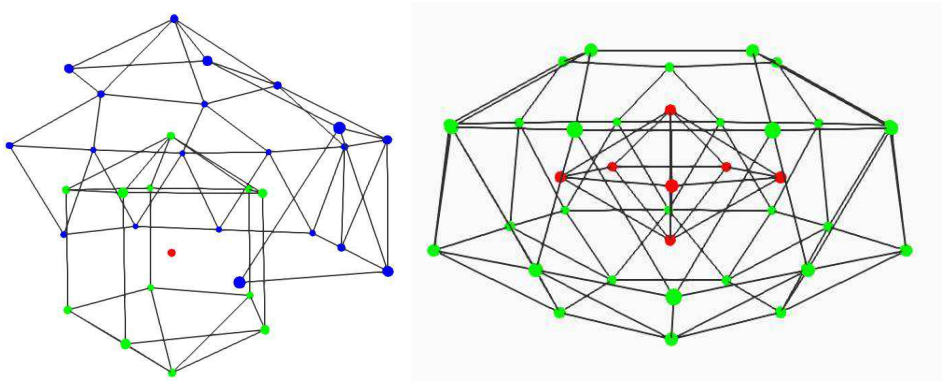
Even with all putative optimal LJ clusters from 2 to 1000 in the lattice IF, I can not prove my conjecture. But, reviewing my previous work and the mathematical properties of the LJ potential function, it is possible to determine from the cubic lattice (CB) all optimal LJ clusters in efficient time.

This paper presents an evolutive algorithm based in our previous Genetic algorithm. It is based on the partial growing sequence property that the optimal LJ clusters exhibe (To my knowledge, it was Northby [12] the pioneer



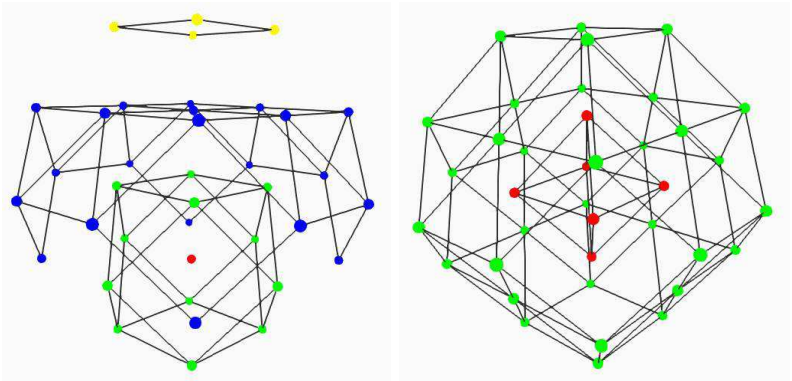
a) b)

Figure 3: a) C_{37}^{*}'s view with nucleus n7 and b) C_{37}^{*}'s view with nucleus n1 IC.



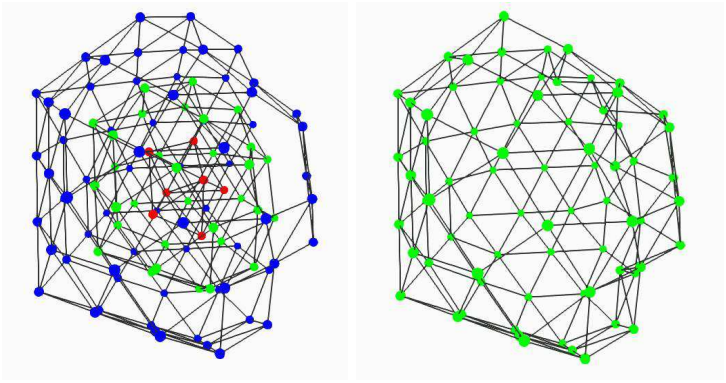
a) b)

Figure 4: a) C_{37}^{*}'s view with nucleus n1 IR and b) non optimal, symmetric C_{37} with nucleus n7 .



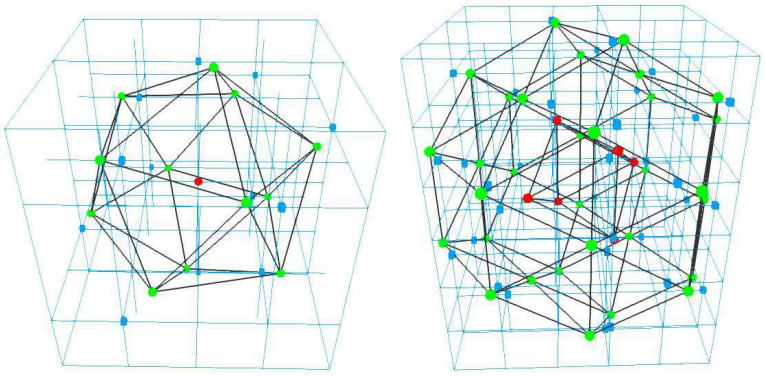
a) b)

Figure 5: a) C_{38}^{*}'s view with nucleus n1, and b) C_{38}^{*}'s classical view with nucleus n6



a) b)

Figure 6: a) C^*_{107} with nucleus n7, b) C^*_{107}'s shell



a) b)

Figure 7: a) C^*_{13} b) C^*_{38} with their initial points inside of CB lattice

to state the growing sequence property of the optimal LJ cluster over the IC lattice, also Hoare [8] pointed out the morphology of the microclusters). It means that clusters with relative closed number of particles could have similar geometry or in other words, they belong to same lattice or they belong to the same geometrical family or they shares some similar bricks or building blocks.

Some ideas and techniques are difficult to replicate, therefore for this article, I added a simple Matlab programs to visualice my novel cluster partition and geometry, and to help for verifying my 8 categories of classification by similar number of particles considered the nucleus.

The corroboration of my results was possible because all the putative optimal LJ clusters are reported in The Cambridge Cluster Database (CCD) [17].

The next subsection depicts the notation used. Section 2 has the properties and the proposition. The subsection 2.1 depicts the technique for the creation of a partition of the cluster's particles into layers, and subsection 2.2 depicts an heuristic for determining a cluster's nucleus (in the appendix a Matlab program of such heuristic is depicted). Section 3 describes my version of parallel evolutionary algorithm. The next section presents the numerical results, and finally, the last section the conclusions and the future work.

1.1 Notation

Given a set S, $|S|$ is the number of elements of the set. Also if $A[\cdot]$ is an array, $|A[\cdot]|$ is the number of elements of the array. $\emptyset$ is the empty set. $||\cdot||$ is the norm in $\mathbb{R}^3$.

Particularly, C_n^* denotes an optimal LJ cluster with n particles, and C_n denotes an arbitrary cluster with n particles.

A cluster C_n or C_n^* are sets of natural numbers, where each number correspond to a particle's properties (p_i). For this research the particle's properties are the particle's 3D coordinates. $||p_i, p_j||$ is the Euclidian distance between particles p_i and p_j.

By example, $C_n^* = \{1, 2\}$, $p_1 = (-\frac{d^*}{2}, 0, 0)$, and $p_2 = (\frac{d^*}{2}, 0, 0)$ where $d^* = \sqrt[6]{2}$ is the optimal distance for two particles under LJ potential:

$$LJ(d) = d^{-12} - 2d^{-6}$$

Several references explain how to build IC and FC lattices [10, 11, 16, 18]. The CB lattice is very simply is the set of points that correspond to the intersection of the parallel lines to the axes with a separation of $d^*/2$ from the (0,0,0).

2 Properties of LJ

There are several articles about LJ potential function's properties. The proposition 1 in [2] is repeated as proposition 2.1 in [3], together with proposition 2.2:

Proposition 2.1 Exist a discrete set, Ω, where $\forall j \in N$, $j \geq 2$, the potential of SOCDXX(j) has the same ("close value") optimal value of SOCCXX(j) for a potential function such that

1. $\lim_{r_{i,j} \to 0} \mathrm{VXX}\left(r_{i,j}\right) = \infty$.
2. $\nabla^2 \mathrm{VXX}\left(x^*\right)$ semi-positive, $\|\nabla \mathrm{VXX}\left(x^*\right)\| \ll 1$ and $\frac{\|\nabla \mathrm{VXX}_{(x^*)}\|}{|\mathrm{VXX}_{(x^*)}|} < \delta_0$, where $0 < \delta_0 \ll 1$

where XX is BU or LJ.

where SOCYXX means search for optimal cluster, D is discrete, C is continues and XX is LJ for Lennard Jones Potential or BU for Buckingham potential.

Proposition 2.2 Any shape of n particles with edges $\approx d^*$ can be approximated from the CB lattice.

This means that with an appropriate region of CB lattice is sufficient to look for optimal clusters of size n. I did not state the size of the appropriate region of CB. However, today, any optimal LJ cluster in the CCD has an initial configuration in CB lattice, such that from this initial configuration converges by a minimization process to its corresponding putative optimal LJ cluster.

Proposition 2.1. *For any set of particles of a cluster's CL or a set of particles of a region RL of any lattice based on a unit u. Then corresponding region RB of the CB lattice such RB covers them under the $||\cdot||_\infty$. Then particles of CL or RL are less than the number of particles of RB, i.e., $|CL| < |RB|$ or $|RL| < |RB|$, where $|\cdot|$ is the number of particles.*

Proof. Under the $||\cdot||_\infty$ any region of CB is a 3D cube. By construction, it has a point at the center $(0,0,0)$, the first cube with $-u/2, 0, u/2$ has 3^3 points, the second cube with $-u, -u/2, 0, u/2, u$ has 5^3 points, ..., the k cube has $(2k+1)^3$ points. Any polyhedra or lattice based in the unit u can not have more than 12 neighbors at ratio u. The icosahedra has 13 points but the corresponding cube to cover it is the second cube, with 5^3 points, i.e., no. particles of icosahedra ¡ no. particles of unit cube of CB lattice. In general, for a given cluster CL or region RL they can be divided and contained by a set of unit cubes of CB, which is a cube, let's call RB. Therefore, $|CL| < |RB|$ or $|RL| < |RB|$. □

It follows that any region of the CB lattice has more points than the same region of a lattice.

But more important, the global continuos optimal LJ cluster can be approximated in a discrete set of 3D points, Ω. Then a connection between RB an appropriate region and Ω will be provide a discrete set of 3D points where the continuous optimal global cluster is approximated by a discrete set of points! A local minimization procedure is the connection to approximate the continuous optimal global in RB. On the other hand, for a cluster with n particles, let's suppose to have an appropriate region RB, $m = |RB|$. The number of the posible clusters of size n in RB is $M = \binom{n}{m} \gg 0$.

Note that M is a big number. It follows naturally from prop. 2.1 than for any region of a given lattice, the number of clusters with n particles is $\ll M$.

Proposition 2.2. *RB is an appropriate search region of the CB lattice for a cluster with n particles, $\mathrm{M} = \binom{n}{m}, m = |RB|$, M is a huge positive number. $|RL|$ is a region of a lattice where there are different clusters with n particles, and it is supposed that it contains the optimal LJ cluster. Then*

$$P\left(\frac{F_1}{RB}\right) < P\left(\frac{F_2}{RB \cup RL}\right)$$

where $P(\cdot)$ is a probability function, F_1 is the set of the optimal candidates for being the global optimal LJ cluster in RB, and F_2 is the set of the optimal candidates for being the global optimal LJ cluster in $RB \cup RL$.

Proof. It follows from

$$|RL| f_1 < f' M$$

where $f_1 = |F_1|$, $f' > 0$ is the number of candidates for being the global optimal LJ cluster in RL, $f' > 0$, it is not zero because the assumption that RL contains the optimal LJ cluster, $f_1 \ll \sqrt{M}$, and $|RL| \ll \sqrt{M}$. Then

$$(M + |RL|) f_1 < (f_1 + f') M,$$

$$P\left(\frac{F_1}{RB}\right) = \frac{f_1}{M} < \frac{f_1 + f'}{M + |RL|} = P\left(\frac{F_2}{RB \cup RL}\right)$$

□

It is important to assume that $F_2 \cap RL \neq \emptyset$, to increase the probability for determining the global optimal clusters, otherwise the probability does not increase. Many of the ad-hoc, heuristic, genetic, and evolutionary algorithms for determining the optimal LJ clusters have been used this property as previous knowledge to favorece some candidates over others with success and speed to replicate the putative optimal LJ clusters.

In a personal communication, I suggested at 2004 to Shao, et al. to use different lattices from [16]. In [15] appears the acknowledge: "The authors would like to thank Prof. Carlos Barrón Romero for his personal communications and collaborations with us in the studies on the lattice-based optimization methods, including also the work published in J. Phys. Chem. A, 108, 3586-3592 (2004)."

So even, knowing that an appropriate region of the CB lattice has the optimal LJ clusters, to improve the efficiency for determining optimal LJ cluster is a good strategy to use other sources of candidates to favorece diversity in the complex process for looking the unknown optimal LJ clusters.

Finally, the theoretical results point out that it is posible to increase the speed of any algorithm for determining optimal LJ clusters but without any proof that they are global optimal. The repeated putative optimal LJ clusters are stationary states, from where a criteria such of the number of times that the same cluster appears, then stop and accept it as the putative optimal global LJ cluster.

The number of steps in these cases are clearly very less than $M = \binom{n}{m}, m = |RB|$. M is the huge number related to the numbers of candidates to compare for determining global optimality in RB. A force brute algorithm for the estimation of the different combinations of a set can be found in [3], it is a version for determining the different cycles of a complete graph, $G = (V, A), |V| = n$.

2.1 Partition technique for a cluster

The geometry of the LJ clusters have been strongly related to different geometric structures (see [9, 8, 12, 16]) icosahedral, dodecahedral, cuboctahedral, and so on.

My segmentation's technique provides different cluster's views as an arbitrary polyhedron with its partitioning into its core, layers and shell by using the particle's neighbors. The advantages to segment a cluster with my technique are 1) to help for interpretation and interaction with other clusters and lattices, and 2) to build a cluster from lego or building blocks.

These properties are quite important because they support the previous research about the knowledge of the clusters' morphology, properties, geometrical families, chemistry, or the well know grow sequence.

A particle's neighbor structure is defined as follow:

1. Define a unit: u.
2. Define a tolerance t as the porcentaje for accepting the expansion and the compression of u. $(0 \leq t \leq 1.0)$.
3. Neighbor's criteria: Particles p_i, p_j are neighbor if an only if $(1-t)u < dist(p_i - p_j) < (1+t)u$.
4. for each particle, $Nvec(i)$ is the number of neighbor of the particle p_i, and $Vec(i,k)$ is the array for storing the number of the particles p_k that they satisfy the neighbor's criteria with a given particle p_i.

where $dist$ is an appropriate distance function between the particles. p_i stands for particle's representation in a n dimensional space, a particle is represented by p_i, which it could contain all the relevant particle's attributes.

For this research, $u = d^*$, p_i is the particle's 3D coordinates, $dist = ||\cdot||$ is the Euclidian distance, and $t = 0.1$.

One characteristic of LJ clusters is the compression-expansion over the distance between particles with respect to the unit d^*. The value of $t = 0.1$ allow to differentiate a diagonal from a expanded-compressed unit u and it works well to identify the "hard LJ optimal clusters" (see [1], by example clusters with 38, 75, 98,75, 76, 77, 102, and 103 particles). For any possible LJ cluster, the upper limit of 12 neighbors over its particles, i.e., $Nvec(i) \leq 12, \forall i$. comes from the upper limit inherited by the 3D twelve kissing spheres geometrical property.

With the cluster's neighbors information, the next algorithm builds an arbitrary partition of a cluster's particles into a set of layers:

Algorithm 2.3. *Partitioning a cluster C_n*
input: *C_n: array of int, for the set of particles' numbers;*
$Nvec$: array of int, with the particles' number of neighbor;
$Vec[i,k]$: array of [int, int] with the particles' neighbors;
$Nuc = \{i_0, i_1, \ldots, i_k\}$: array of int, for a given set of particles's number to be the nucleus, with $|Nuc| \leq n$;
output: *capa: array of int, for the corresponding layer of a particle;*
ncapa: int, for the cluster's number of layers;
memory: *fmk: int;*

---

for *i := 1* **to** *n* **do**
  capa$[i] := 0$;
end for
ncapa $:= 1$;
for *i := 1* **to** $|Nuc|$ **do**
  capa$[Nuc[i]] :=$ *ncapa*

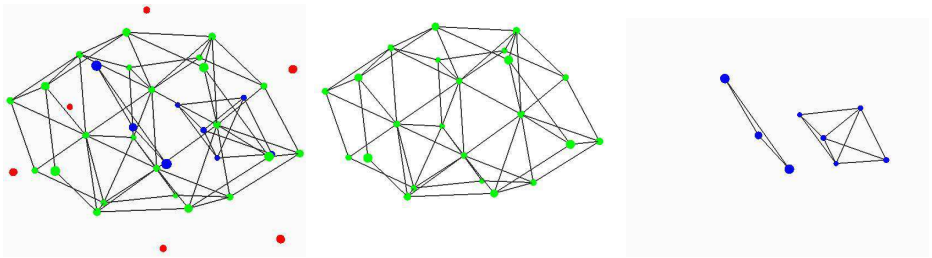


Figure 8: C^*_{37} with its layers for an arbitrary selection of its nucleus

```
end for
fmk := 0;
while (1) do
    for i:=1 to n do
      if (capa[i] == ncapa) then
      for jv := 1 to Nvec[i] do
          kv := Vec[i][jv];
          if (capa[kv] == 0) then
              capa[kv] := ncapa + 1;
               fmk := 1;
          end if
      end for
    ncapa := ncapa + 1;
end while
ncapa := ncapa - 1;
return;
```

Hereafter, layer number 1 is the core or nucleus, and the last layer *ncapa* is the shell.
It is easy to verify that the set *capa* of the particles' numbers is a partition of C_n, i.e,:

- $\bigcup_{i=1}^{ncapa} capa[i] = C_n$
- $capa[i] \cap capa[j] = \emptyset$, $i \neq j$.

The previous algorithm gives an arbitrary cluster partition that it could not correspond to the standard accepted geometric structures but it can be used for genetic cuts for creating a new offspring as playing with set of figures of lego. In particular, the results could be similar to the Hoare's (see [8]) morphology of simple microclusters, polyhedral structures (PT), and an arbitrary representation of cluster's isomeros. Figure 8 depicts C^*_{37} with its layers for an arbitrary selection of its nucleus. Figure 6 depicts C^*_{107} with nucleus n7 and its shell.

2.2 Heuristic for determining a nucleus for a cluster

The proposed heuristic is simple and it is based in previous knowledge of the LJ cluster structures that other authors have been point out.

The main concept is to look for a set of cluster's particles inside of an sphere with center at the cluster's center of mass with ratio $1.1d^*$.

The particles inside of the sphere are natural candidates for being considering the cluster's nucleus. There many cases, for the selection of the cluster's nucleus. Let PN be the set of particles inside of the sphere, and cm the cluster's coordinates of its center of mass:

1. IC or IR when $\exists\ p_k \in PN$, such that $\arg k = min_k||p_i - cm||$, and $||p_k - cm|| < 0.35d^*$. By example, $C^*_1 3, C^*_5 5, \ldots$ are IC (n1 IC), and $C^*_7 5, C^*_7 6, \ldots$ are IR (n1 IR).

2. IC without a particle as a center when $|PN| = 12$ and these 12 are closed to the sphere's shell. This is the case for IC nucleus with 12 particles (n0 IC). By example, $C_5^*21, C_5^*33, \ldots$.

3. When $3 \leq |PN|$ and $|PN \leq 7$, PN is considering the cluster's nucleus. This criteria gives a nucleus with 3 to 7 particles. By example, $n3$: 665, 668, 672, 673, 728, ...; $n4$: 26, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 98, ...; $n5$: 22, 23, 24, 25, 28, 29, 33, 34, 78, ...; $n6$: 31, 32, 38, 43, 44, 99, 121, ...; $n7$: 18, 19, 20, 21, 27, 30, 35, 36, 37, 39, ...

4. when $|PN| \geq 8$, adjust the center of the sphere to the center of mass of mass of the the cluster with the PN's particles with 12 neighbors. The new sphere's ratio is set to $0.9d^*$, then take as the nucleus the particles inside of this new sphere.

It is showed in the appendix the Matlab routine "S_plot_geCl_LJ.m". It is a version of an algorithm using this heuristic. Figure 6 depicts the results of the C_{107}^* and its shell with algorithm 2.3 with a nucleus defined by the heuristic of this section.

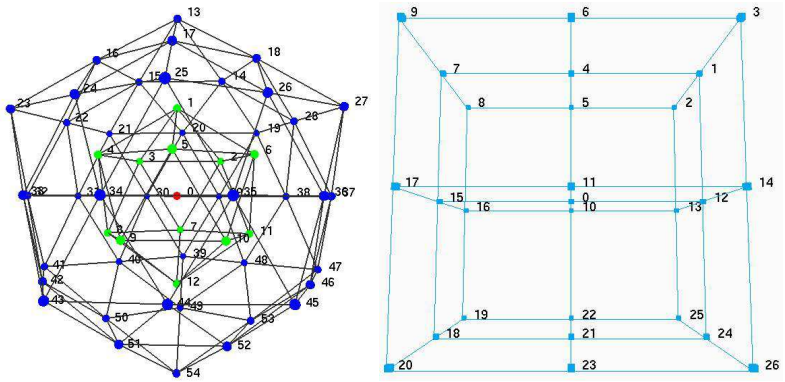
The next algorithm builds a set of coordinates or give a set of number that they correspond to a cluster inside of a region. A region could be and arbitrary set of points, or points of a lattice, or the points of other big cluster.

Algorithm 2.4. *Matching a cluster C_n with a given region R*
input:
p_n: array of 3D, for the particles' coordinates of the cluster C_n;
R_k: array of 3D, with the points' coordinates of the region R;
M: int, with the number of points of the region R;
output:
$r[\cdot]$: array of int, for the corresponding particles' numbers in the R;
$s[\cdot]$: array of 3D, for the closed corresponding particles' coordinates of the points of R;
memory:
d_{min}: real; // minimum distance i_{min}: int; // particle' number $mk[\cdot] := 0$: array of int, set all to 0;

---

if $M < n$ **then**
  print*("Error, it is insufficient the number of points of R for the cluster");*
  return*;*
end if
for $i := 1$ **to** n **do**
  $d_{min} := 10^8$*;*
  for $k := 1$ **to** M **do**
    if *($ml[k] == 0$)* **then**
      $d := dist(p[i], R[k])$*;*
      if *($d < d_{min}$)* **then**
        $d_{min} := d$*;*
        $i_{min} := k$*;*
      end if
    end if
  end for
  $mk[i_{min}] := 1$*;*
  $r[i] := i_{min}$*;*
  $s[i] := R[i_{min}]$*;*
end for
return*;*

The previous algorithm always answers with a set of points and with a set on particles' numbers that they correspond to a cluster, but the original and the output cluster from the region R could have very different shapes. By example, when a cluster is centered at (0,0,0), and the region is box $[20, 50] \times [20, 50] \times [20, 50]$ of the cb lattice. On the other hand, figure 7 depicts C_{13}^* and C_{38}^* inside of a CB region, where the light blue small boxes are their corresponding points of CB lattice.



a) b)

Figure 9: Examples of numeration from the nucleus to its shell a) region of the IC lattice, and b) region of the CB lattice

3 Parallel evolutionary algorithm for searching optimal LJ clusters

The novelty of the Parallel evolutionary algorithm of this section is not a new complete paradigm, as I mentioned before, it is a reload version of previous ad-hoc and genetic algorithm (see [7, 4, 5, 6, 14, 13, 2, 3]).

The term evolutionary algorithm for my approach is justified by the fact that the results are converted into input data, and this cause a change of the expected behavior of the program beyond of its programming. What, I precisely mean is that the efficacy and efficiency of the program for determining optimal LJ clusters is improved. Also, I added new routines based in phenotype and genotype strategies that my previous algorithms have not. But in the essence, it is an evolutionary program improved by his creator to increase its efficiency and efficacy with adding changes into its old routines by hand. One of the aspect to point out, is that previous version was only based in elitism, here the diversity is favored and it will come from the data of the optimal clusters and for the data of the CB lattice, particularly.

The algorithm [14]) now includes the following genotype and phenotype mechanisms.

For the genotype mechanisms, a telephone model for the clusters consist to get a set of number to represent a cluster. This can be done with a region of a lattice and a cluster by using the algorithm 2.4.

An enumeration from the nucleus to its shell can be done by ordering the particles of a region by its ratio, y coordinate and its angle on the XY plane. Figure 9 depict a IC and CB regions with this numeration. This helps because for a cluster, lower number are in the core, larger number are in the shell whatever it is respect to a lattice or to other C_n^*.

With the telephone model for a cluster, a mutation is like to dial the cluster's telephone with one or more mistakes. The mistake numbers can be replaced by any number not in the cluster's telephone with the condition that such numbers are the indices of particles' coordinates in a given region.

Children can be created by replacing sequences of the clusters' telephones of 2 or more parent clusters.

After the creation of the children by any genetic mechanism, a minimization procedure is applied for the corresponding coordinates of the particles' numbers of the children to get a local minimal LJ cluster for elitism selection.

On the other hand, the previous genetic algorithm adds mechanisms to use the algorithm 2.3 with or without the heuristic given in subsection 2.2. New kind of mutations are incorporate by using the matching algorithm 2.4 to transform a cluster into a CB, IC, IF or any lattice before crossover and make up. Previously, the current population include the optimal LJ cluster, the cluster with more 12 neighbors, and the worst LJ cluster. The change is to include the lower and as many clusters as possible of the 8 categories of the heuristic for determining the nucleus with the current optimal LJ cluster.

The parrallel algorithm defines a player main routine, which consists in two main routines: Cerberus and Prometheus.

Algorithm 3.1. *Player*
input:
timer: set an interval of time for sending a stop signal.
I_n*: int parameter of the initial cluster* (≥ 13)*;*
F_n*: int parameter of final cluster* (≥ 13 *and* ($\geq I_n$))*;*
P_{sz}*: int parameter of the population size* (≥ 9)*.*
R_{CB}*: set of 3D points of the CB lattice* ($\gg F_n$)*;*
$R_{L1}, \ldots R_{Lk}$*: set of 3D points of other lattices* ($\gg F_n$)*;*
output:
memory:
C_n^**: private data of the current putative optimal LJ clusters;*

---

while *(1)* **do**
execute *Cerberus;*
execute *Prometheus*($I_n, F_n, P_{sz}, R_{CB}, R_{L1}, \ldots R_{Lk}$)*;*
a timer or the user send *a signal to stop;*
end while

Cerberus is an elitism routine for communicating and keeping the best putative optimal LJ clusters. It take care of the communication but never interrupt the process of Prometheus.

Algorithm 3.2. *Cerberus*
input:
P_c*: input pile of messages for* C_k *(LJ clusters);*
st_P*: int, exclusive variable to communicate with Prometheus's state, 1: Prometheus is searching or 0:Prometheus is not searching;*
output:
signal: semaphore command for waiting or executing;
memory:
C_n^**: private data of the current putative optimal LJ clusters;*

---

signal *Prometheus* **goes***;*
while *(1)* **do**
if *(*$st_P == 0$*)* **then**
while *pile(*P_c*) is not empty* **do**
signal *Prometheus* **to wait***;*
C_k *:= pop(*P_c*);*
if $LJ(C_k) < LJ(C_k^*)$ **then**
$(C_k^*) = (C_k)$*;*
send *message* C_k^* *to others players;*
end if
end while
signal *Prometheus* **to continue***;*
end while

Prometheus is the implementation of the previous evolutionary algorithm. It has exclusive access to the best LJ clusters during the evolutionary process.

Algorithm 3.3. *Prometheus*
input:
I_n*: int parameter of the initial cluster* (≥ 13)*;*
F_n*: int parameter of final cluster* (≥ 13 *and* ($\geq I_n$))*;*
P_{sz}*: int parameter of the population size* (≥ 9)*.*
R_{CB}*: set of 3D points of the CB lattice* ($\gg F_n$)*;*
$R_{L1}, \ldots R_{Lk}$*: set of 3D points of other lattices* ($\gg F_n$)*;*
signal: semaphore command for waiting or executing;
output:
st_P*: int, exclusive variable to communicate its state, 1: busy or 0:waiting;*

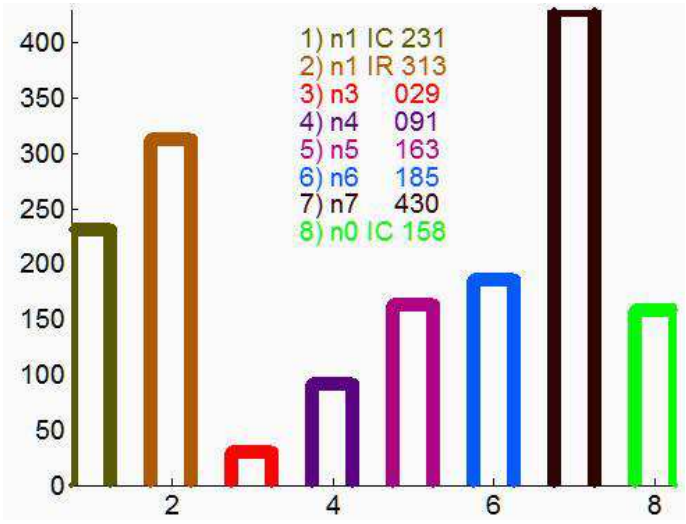


Figure 10: Histogram of nucleus type for C_n^*, $n = 13, \ldots, 1612$ particles

memory:
C_n^*: private data of the current putative optimal LJ clusters;

---

while *(1)* **do**
  st_P : = 0;
  for $n := I_n$ **to** F_n **do**
    do *Cerberus(signal) or player(signal);*
    st_P := 1;
    execute: *evolutionary algorithm for exploring C_n*
    st_P :=0;
  end for
end while

When Prometheus is executing the evolutionary algorithm, there is not access to the private memory even for others clusters different of the current n. This is because the evolutionary algorithm could use any C_j^* for creating offsprings at any time. Before or after, the process of the evolutionary algorithm, or when Prometheus is off, there is access to the best LJ optimal clusters.

The player routine is designed for working with copies of it. This could cause a bootle's neck for the communications. Therefore, it is convenient to define a master player. In this case, only the master has the ability to send and receive messages, meanwhile the slave players can only send messages to it.

4 Results

My previous results [2] are in the figure 1. It depicts a set of particles MIF1739, which contains C_n^*, $n = 2, \ldots, 1000$. I tried to use MIF1739 has a main lattice from where an algorithm could takes advantage of its building property: $\exists\, C_n \in$ MIF1739, such that by a minimization process, C_n converges to C_n^*. However, it is not easy task to locate a "good" initial set of points closed to an optimal LJ cluster. Figure 2 depicts where C_{38}^* and C_{664}^* are located into the IF lattice. It is possible to select points by using sphere in MIF1739. Two parameters are need, the ratio and the center of sphere.

The efficiency of the evolutionary algorithm changes dramatically with the incorporation of the CB lattice, and the phenotype and genotype strategies. The best results comes from starting with no optimal clusters but by using CB lattice and IC, IR, FC, dodecahedral lattices, and 14 as the size of the population.

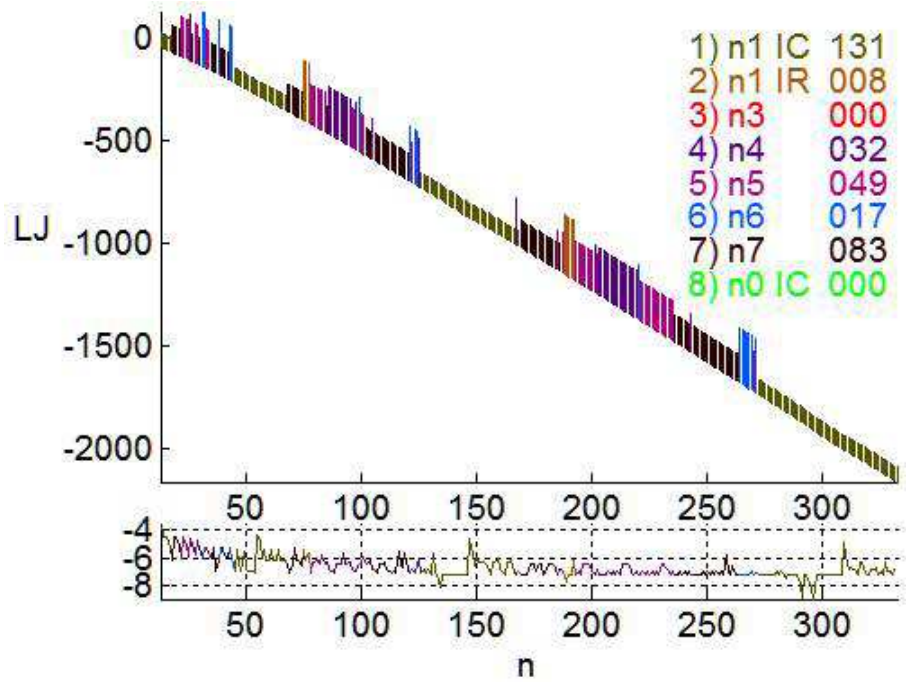


Figure 11: LJ potential, potential difference vs C_n^*, $n = 13, \ldots, 332$ particles

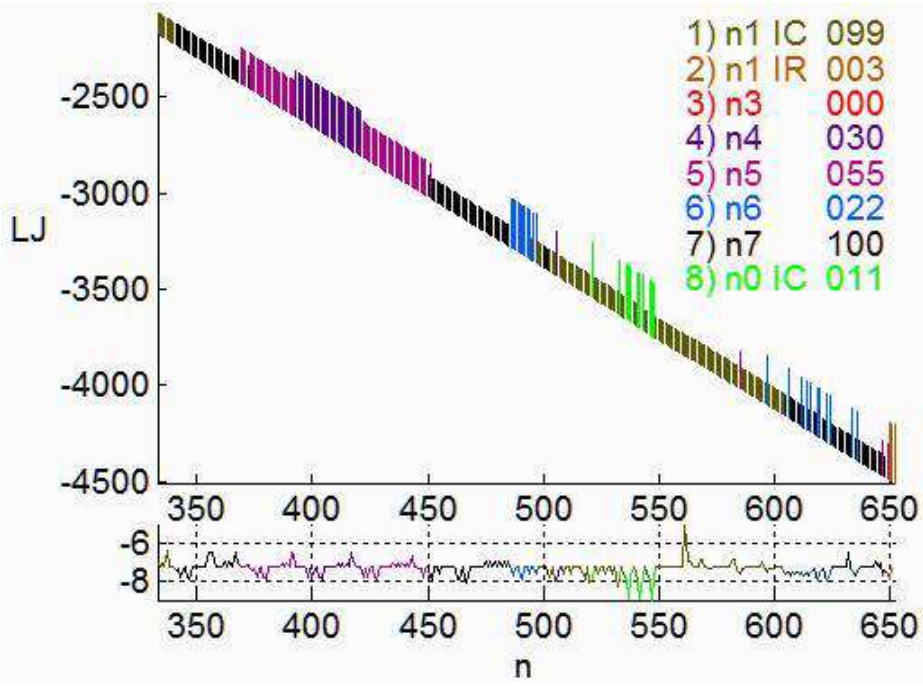


Figure 12: LJ potential, potential difference vs C_n^*, $n = 333, \ldots, 652$ particles

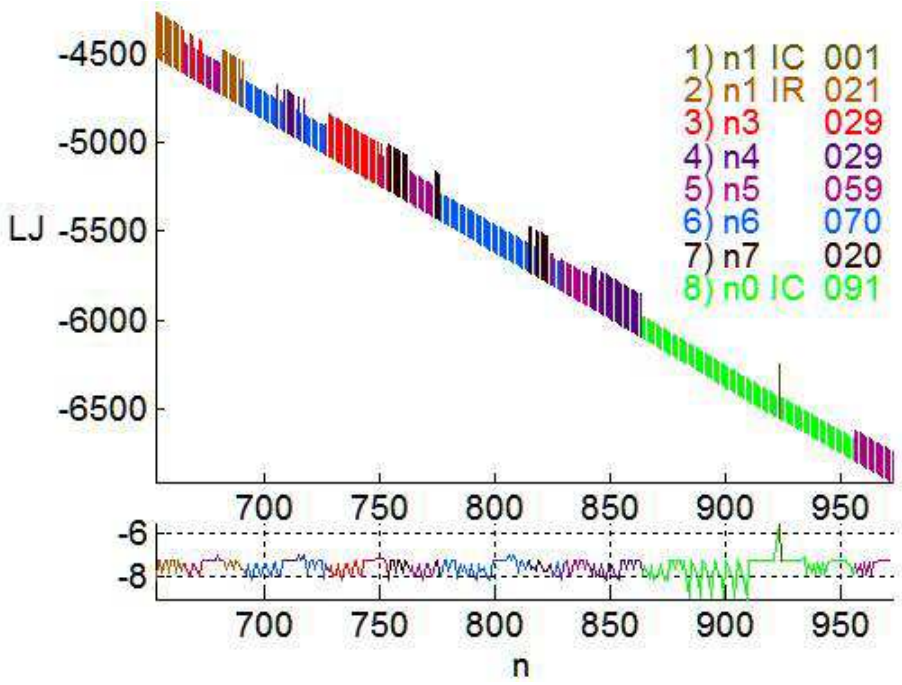


Figure 13: LJ potential, potential difference vs cluster with C_n^*, $n = 653, \ldots, 972$ particles

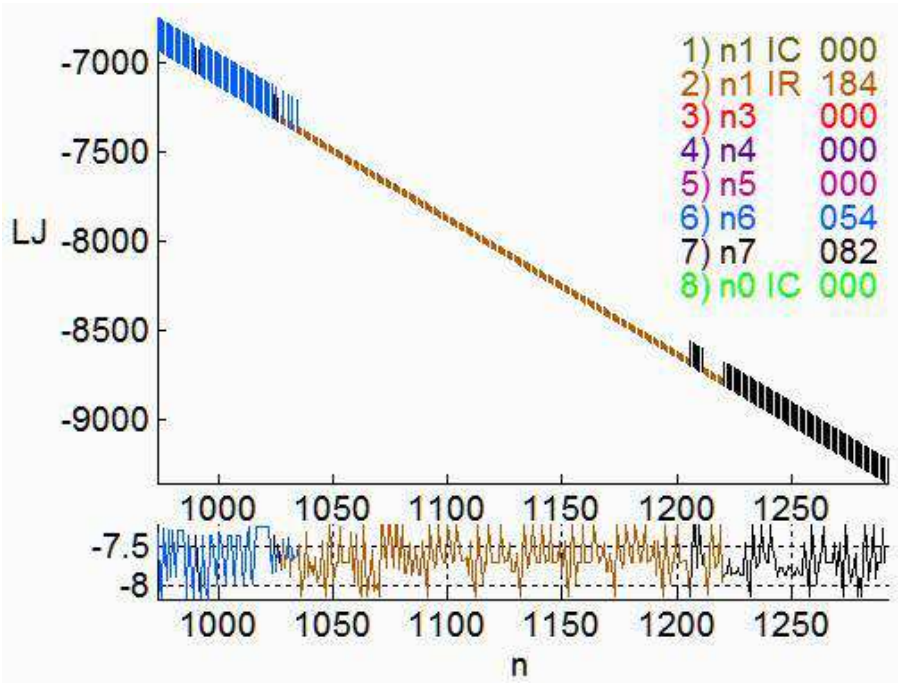


Figure 14: LJ potential, potential difference vs C_n^*, $n = 973, \ldots, 1292$ particles

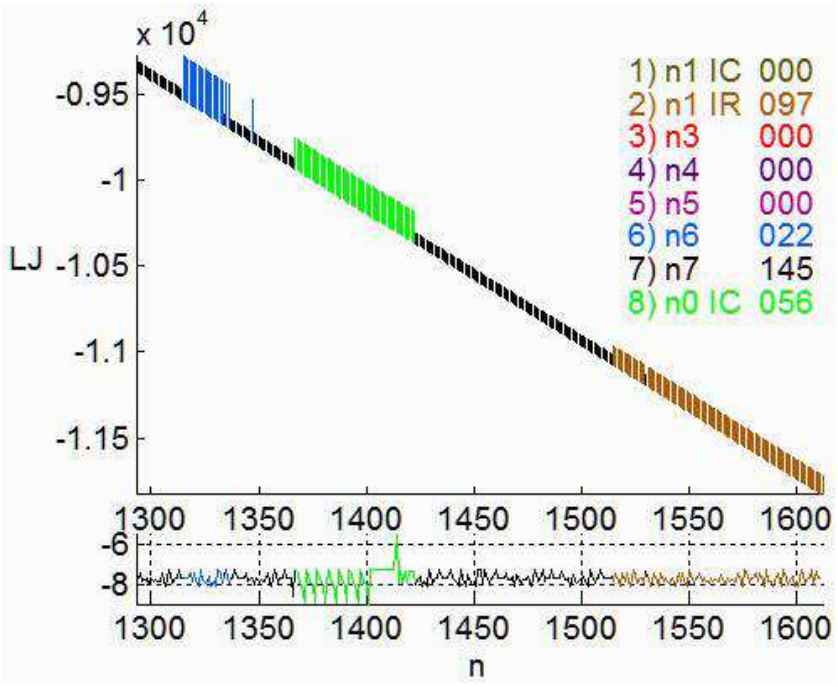


Figure 15: LJ potential, potential difference vs C_n^*, $n = 1293, \ldots, 1612$ particles

The heuristic for determining a nucleus (see subsection 2.2) and the algorithm 2.3, helped to extend the selection and interaction between clusters to create offspring for mutation or phenotype crossover or genotype crossover. This heuristic classifies into 8 categories by just using the numbers of particles in a nucleus. The nucleus types n4, n5, n6, and n7 are not geometrically equal. A refinement of heuristic is possible, but it has a computation cost.

Figure 10 depicts the histogram of 8 categories resulting of this heuristic for the C_n^*, $n = 13, \ldots, 1612$. Tables 1, 2, 3, and 4 contains the classification of the clusters. It seems that many cases of C_n^* are obtained rapidly by a the make up operation of its previous or next clusters, but also by considering to extend the diversity of the current population to 8 categories.

My results could help to answer some old conjetures about the morphology of the microclusters. See Hoare [8]: "Werfelmer's essential contribution was to point out the possibility of extremely compact fivefold symmetric structures for N7, suggesting that the pentagonal bipyrimid (N=7) (fig.3(a)) and the icosahedron (N=13) (fig.3(b)) might be the dominant motifs in larger assemblies." It is partially true, from table 4the type 7), a nucleus with 7 particles (a pentagonal bipyramid) is the dominant motif for C_n^*, $n = 18, \ldots, 1530$, but IC is not a dominant motif from table 1, type 1) and type2) without considering type 8) (a nucleus IC with 12 particles, which was unknown at 1983).

Figures 11, 12, 13, 14, and 15 depict where the different nucleus type appears. At the bottom of each figure the LJ potential difference bet the consecutive clusters is depicted. Some type of optimal clusters are isolated and the LJ potential difference is highly variable from $n = 13$ to 1420. But after this cluster it seems to diminish its variations for the IR C_n^*, $n \geq 142$. My results are 1600 optimal LJ clusters with $n = 13, \ldots, 1612$ particles, (Most of them are posted in The Cambridge Cluster Database (CCD) [17]), a novel 8 categories of nucleus classification, and 65 new putative LJ Clusters, which are not reported at December of 2016. See table 5.

5 Conclusions and future work

The advances of the technology and science of Physics and Chemistry are fantastic, together with the molecular and the nanostructures design. The results presented here have many implications for the computational molecular design and their models and algorithms.

I hope to witness, that it is quite possible to replicate and to improve these results by using one of the top worldwide supercomputer. Some of the definitions are broad, and this research can be easily extended and applied for exploring geometries and interactions of clusters under other molecular potentials.

Appendix

Matlab Programs

```
function  S_plot_Cl_LJ(ncl,xcl,ycl,zcl,nv1,nv2)
% This subroutine draws the geometry of
% a minimal Lennard Jones Potential's cluster
% The input parameters are:
% ncl : numbers of particles
% xcl, ycl, zcl: arrays of numbers corresponding to the 3D
% cluster's coordinates
% nv1, nv2 : integer number to determine the shells to draw
% With nv1=0 and nv2=2, the cluster's nucleus and the first shell
% are depicted (layer 1 is the nucleus).
% ========================================================================
% More information of this subroutine is in the article:
% Discrete Optimal Global Convergence of a Evolutionary Algorithm
% for Clusters under the  Potential of Lennard Jones
% Author: Carlos Barron-Romero
% Universidad Autonoma Metropolitana, campus Azcapotzalco
% Mexico City.
% This subroutine can be freely used, distributed or modified.
% ========================================================================
% Compute center of mass
xclm=mean(xcl);
yclm=mean(ycl);
zclm=mean(zcl);
% Arrays for particle's neighbors and number of neighbors
vec=zeros(ncl,12);
nvc=zeros(ncl,1);
% dmg is the optimal distance of a pair of particles under
% Lennard Jones Potential
dmg=2^(1/6);
% 10% is the factor to define the lower and upper limits
% for accepting a particle's neighbor
tol=0.1;
d_inf = dmg * (1 - tol);
d_sup = dmg * (1 + tol);
%
% This loop determines the particle's neighbor
for i=1:ncl-1
    for j=i+1:ncl
dij=norm([(xcl(i)-xcl(j)),(ycl(i)-ycl(j)),(zcl(i)-zcl(j))]);
        if ((d_inf < dij) && (dij < d_sup))
            nvc(i)=nvc(i)+1;
            vec(i,nvc(i))=j;
            nvc(j)=nvc(j)+1;
            vec(j,nvc(j))=i;
        end
    end
```

```
end
% Select a set of particles closed to the cluster's center of mass
ra = dmg*1.1;
pnuc=zeros(13,1);
nnuc=0;
fnuc = 0;
for i=1:ncl
    dcl=norm([(xcl(i)-xclm),(ycl(i)-yclm),(zcl(i)-zclm)]);
    if (dcl < ra)
        nnuc=nnuc+1;
        pnuc(nnuc)=i;
    end
end
% Analyze the set of particles
if (nnuc >0)
    % First case.
    % Look for a particle with 12 neighbors
    % closed to the CM
    inuc = -1;
    d12nuc = 99999.999;
    for k=1:nnuc
        i=pnuc(k);
        if (nvc(i) == 12)
dcl=norm([(xcl(i)-xclm),(ycl(i)-yclm),(zcl(i)-zclm)]);
            if (dcl < d12nuc)
                d12nuc = dcl;
                inuc=i;
            end
        end
    end
    ra_nuc = dmg * 0.35;
    if ((inuc ~= - 1) & (d12nuc < ra_nuc))
        % There is a particle with 12 neighbors
        pnuc(1) = inuc;
        nnuc = 1;
        ra = d12nuc;
        fnuc = 1;
    end
    % After verify that there is no center,
    % Then it is the nucleus with 12 particles
    if ((inuc == - 1) & (nnuc == 12))
        fnuc = 1;
    end
end
% Final case.
% Skip four (tetrahedron, nnuc=4),
% five (Trigonal bipyramid, nnuc=5),
% six particles (octahedron, nnuc=6),
% (pentagonal polyhedron bipyramide, nnuc=7)
%
if ((fnuc == 0) & (nnuc >= 8))
    % Adjust the cluster's center of mass
    % considering only particles with 12 neighbors
    % of the selected set pnuc
```

```
    nclm = 1;
    for k=1:nnuc
        i=pnuc(k);
        if (nvc(i) == 12)
            xclm = xclm + xcl(i);
            yclm = yclm + ycl(i);
            zclm = zclm + zcl(i);
            nclm = nclm + 1;
        end
    end
    xclm = xclm / nclm;
    yclm = yclm / nclm;
    zclm = zclm / nclm;
    % Adjust the selected set, keeping the closed
    % to the adjusted center
    ra = dmg*0.9;
    pnuc_nw=zeros(13,1);
    nnuc_nw=0;
    for k=1:nnuc
        i=pnuc(k);
        dcl=norm([(xcl(i)-xclm),(ycl(i)-yclm),(zcl(i)-zclm)]);
        if (dcl < ra)
            nnuc_nw=nnuc_nw+1;
            pnuc_nw(nnuc_nw)=i;
        end
    end
    % Take this new set as the nucleus
    pnuc = pnuc_nw;
    nnuc = nnuc_nw;
    fnuc = 1;
end
% Determine the cluster's layers
% with the nucleus particles
capa=zeros(ncl,1);
ncapa=1;
for jp=1:nnuc
    capa(pnuc(jp))=1;
end
while (1)
    fmk=0;
    for i=1:ncl
        if (capa(i) == ncapa)
            for jv=1:nvc(i)
                pvc=vec(i,jv);
                if (capa(pvc)== 0)
                    capa(pvc) = ncapa+1;
                    fmk=1;
                end
            end
        end
    end
    if (fmk == 0)
        break;
    end
```

```
    ncapa = ncapa + 1;
end
% Color table
tclr = [ 1,0,0; ...
    0,1,0; ...
    0,0,1; ...
    1,1,0; ...
    51/255, 153/255, 1; ...
    1,0,1; ...
    0.5,0.5,1; ...
    0.5,0.5,0.5; ...
    1,0.5,1; ...
    1,0.5,0.5; ...
    1,0.5,0.75; ...
    1,0.75,0; ...
    0,0,0];
hold on;
for i=1:ncl
    if (capa(i) < nv1)
        continue;
    end
    if (capa(i) > nv2)
        continue;
    end
    % cluster's lines
    for jv=1:nvc(i)
        pvc=vec(i,jv);
        if (capa(i) == capa (pvc))
            line([xcl(i),xcl(pvc)], ...
                [ycl(i),ycl(pvc)], ...
                [zcl(i),zcl(pvc)], ...
                'Color',tclr(capa(i),:), ...
                'LineWidth',1);

        end
    end
    % particles
    plot3(xcl(i), ...
        ycl(i), ...
        zcl(i), '-ko',...
        'LineWidth',1,...
        'MarkerEdgeColor','k', ...
        'MarkerFaceColor',tclr(capa(i),:),...
        'MarkerSize',8);
end
axis equal;
grid on;
linp=sprintf('Cluster of %d particles',ncl);
title(linp);
view(45,45);
hold off;

function [n,x,y,z] = S_read_Cl_LJ(file_name)
% This subroutine reads in the format of the file from the
```

```
% The Cambridge Energy Landscape Database (\protect\vrule width0pt\protect\href{http://www-wales.ch.cam
% of a minimal cluster under Lennard Jones Potential
%
% The input parameters is the file name
% Is is ####.txt, where #### is the cluster's number of particles
%
% ========================================================================
% This subroutine is in the article:
% Discrete Optimal Global Convergence of a Evolutionary Algorithm
% for Clusters under the  Potential of Lennard Jones
% Author: Carlos Barron-Romero
% Universidad Autonoma Metropolitana, campus Azcapotzalco
% Mexico City.
% This subroutine can be freely used, distributed or modified under
% your own responsibility.
% ========================================================================
%
fid=fopen(file_name);
p = fscanf(fid,'%g %g %g', [3 inf]);
fclose(fid);
% x, y and z are the cluster's coordinates
x=p(1,:);
y=p(2,:);
z=p(3,:);
% n is the cluster's number of particles
n=length(x);

% This program calls the
% subroutine S_plot_geCl_LJ_cl to draw the geometry of
% an optimal Lennard Jones cluster
% ========================================================================
% More information of this subroutine is in the article:
% Discrete Optimal Global Convergence of a Evolutionary Algorithm
% for Clusters under the  Potential of Lennard Jones
% Author: Carlos Barron-Romero
% Universidad Autonoma Metropolitana, campus Azcapotzalco
% Mexico City.
% This subroutine can be freely used, distributed or modified under
% your own responsibility.
% ========================================================================
feature('UseGenericOpenGL',0);
[filename,pname] = uigetfile('*.TXT');
% Define your own routine to read the particles' coordinates
% of a optimal cluster under the Leenard Jones Potential
% or S_read_cl_LJ is set to read the files in the
% The Cambridge Energy Landscape Database (\protect\vrule width0pt\protect\href{http://www-wales.ch.cam
%
% The input parameters is the file name
% Is is ####.txt, where #### is the cluster's number of particles
[ncl, xcl,ycl,zcl] = S_read_Cl_LJ([pname,filename]);
nv1=0;
nv2=2;
clf;
S_plot_geCl_LJ(ncl,xcl,ycl,zcl,nv1,nv2);
```

n1 IC 231	**n1 IR** 313
13 14 15 16 17 45 46 47 48 49	75 76 77 188 189 190 191 192 650 651 652 653 654 655
50 51 52 53 54 55 56 57 58 59	656 657 658 659 660 661 662 663 664 682 683 684 685
60 61 62 63 64 65 66 67 126	686 687 688 689 691 1027 1029 1031 1033 1035 1036
127 128 129 130 131 132 133	1037 1038 1039 1040 1041 1042 1043 1044 1045 1046
134 135 136 137 138 139 140	1047 1048 1049 1050 1051 1052 1053 1054 1055 1056
141 142 143 144 145 146 147	1057 1058 1059 1060 1061 1062 1063 1064 1065 1066
148 149 150 151 152 153 154	1067 1068 1069 1070 1071 1072 1073 1074 1075 1076
155 156 157 158 159 160 161	1077 1078 1079 1080 1081 1082 1083 1084 1085 1086
162 163 164 165 166 168 272	1087 1088 1089 1090 1091 1092 1093 1094 1095 1096
273 274 275 276 277 278 279	1097 1098 1099 1100 1101 1102 1103 1104 1105 1106
280 281 282 283 284 285 286	1107 1108 1109 1110 1111 1112 1113 1114 1115 1116
287 288 289 290 291 292 293	1117 1118 1119 1120 1121 1122 1123 1124 1125 1126
294 295 296 297 298 299 300	1127 1128 1129 1130 1131 1132 1133 1134 1135 1136
301 302 303 304 305 306 307	1137 1138 1139 1140 1141 1142 1143 1144 1145 1146
308 309 310 311 312 313 314	1147 1148 1149 1150 1151 1152 1153 1154 1155 1156
315 316 317 318 319 320 321	1157 1158 1159 1160 1161 1162 1163 1164 1165 1166
322 323 324 325 326 327 328	1167 1168 1169 1170 1171 1172 1173 1174 1175 1176
329 330 331 332 333 334 335	1177 1178 1179 1180 1181 1182 1183 1184 1185 1186
336 337 338 339 340 495 498	1187 1188 1189 1190 1191 1192 1193 1194 1195 1196
499 503 504 505 507 508 509	1197 1198 1199 1200 1201 1202 1203 1204 1205 1212
510 511 512 513 514 515 516	1213 1214 1215 1216 1217 1218 1219 1220 1515 1516
517 518 519 520 522 523 524	1517 1518 1519 1520 1521 1522 1523 1524 1525 1526
525 526 527 528 529 530 531	1527 1528 1529 1531 1532 1533 1534 1535 1536 1537
532 534 535 539 540 544 545	1538 1539 1540 1541 1542 1543 1544 1545 1546 1547
549 550 551 552 553 554 555	1548 1549 1550 1551 1552 1553 1554 1555 1556 1557
556 557 558 559 560 561 562	1558 1559 1560 1561 1562 1563 1564 1565 1566 1567
563 564 565 566 567 568 569	1568 1569 1570 1571 1572 1573 1574 1575 1576 1577
570 571 572 573 574 575 576	1578 1579 1580 1581 1582 1583 1584 1585 1586 1587
577 578 579 580 581 582 583	1588 1589 1590 1591 1592 1593 1594 1595 1596 1597
584 586 587 588 589 590 591	1598 1599 1600 1601 1602 1603 1604 1605 1606 1607
592 593 594 595 596 598 599	1608 1609 1610 1611 1612
600 601 602 603 604 923	

Table 1: Type 1 and 2 of the $C_n^*, n = 13, \ldots, 1612$

References

[1] Conquering the hard cases of lennard-jones clusters with simple recipes. *Computational and Theoretical Chemistry*.

[2] C. Barrón-Romero. Minimum search space and efficient methods for structural cluster optimization. *arXiv*, Math-ph:0504030-v4, 2005. To honor the CIMAT's XXV Anniversary.

[3] C. Barrón-Romero. The Complexity of the NP-Class. *arXiv*, arxiv.org/abs/ 1006.2218, 2010.

[4] C. Barrón-Romero, S. Gómez, and D. Romero. Archimedean Polyhedron Structure Yields a Lower Energy Atomic Cluster. *Applied Mathematics Letters*, 9(5):75–78, 1996.

[5] C. Barrón-Romero, S. Gómez, and D. Romero. Lower Energy Icosahedral Atomic Cluster with Incomplete Core. *Applied Mathematics Letters*, 10(5):25–28, 1997.

[6] C. Barrón-Romero, S. Gómez, D. Romero, and A. Saavedra. A Genetic Algorithm for Lennard-Jones Atomic clusters. *Applied Mathematics Letters*, 12:85–90, 1999.

n3 29	**n4** 91
665 668 669 672 673	26 86 87 88 89 90 91 92 93 94 95 98 125 167 201 203 204 205 206
728 729 730 731 732	207 208 209 210 211 212 213 214 215 216 217 218 219 393 394
733 734 735 736 737	395 396 397 398 399 400 401 402 403 404 405 406 407 408 409
738 739 740 741 742	410 411 412 413 414 415 416 417 418 419 420 421 506 706 709
743 744 745 746 747	710 711 712 713 715 717 842 843 844 846 847 848 849 850 851
748 749 751 753	852 853 854 855 856 857 858 859 860 861 862 863

Table 2: Type 3 and 4 of the $C_n^*, n = 13, \ldots, 1612$

n5 163	**n6** 185
22 23 24 25 28 29 33 34 78 79 80 81	31 32 38 43 44 99 121 123 124 220 264 265 266
82 83 84 96 97 100 101 105 122 185	267 268 269 271 486 487 488 489 490 491 492 493
187 193 194 195 196 197 198 199 200	494 496 497 597 606 612 614 616 619 620 623 624
202 221 222 223 224 225 226 227 228	634 636 690 692 693 694 695 696 697 698 699 700
229 230 231 232 233 234 235 243 270	701 702 703 704 705 707 708 714 716 718 719 720
369 370 371 373 374 375 376 377 378	721 722 723 724 725 726 777 778 779 780 781 782
379 380 381 382 383 384 385 386 387	783 784 785 786 787 788 789 790 791 792 793 794
388 389 390 391 392 422 423 424 425	795 796 797 798 799 800 801 802 803 804 805 806
426 427 428 429 430 431 432 433 434	807 808 809 810 811 812 813 814 817 826 827 828
435 436 437 438 439 440 441 442 443	973 974 975 976 977 978 979 980 981 982 983 984
444 445 446 447 448 449 451 585 647	985 986 987 988 989 992 993 994 995 996 997 998
649 666 667 670 671 674 675 676 677	999 1000 1001 1002 1003 1004 1005 1006 1007
678 679 680 681 727 750 752 763 764	1008 1009 1010 1011 1012 1013 1014 1015 1016
765 766 767 768 769 770 771 772 773	1017 1018 1019 1020 1021 1022 1023 1025 1028
824 825 829 830 831 832 833 834 835	1030 1032 1034 1315 1316 1317 1318 1319 1320
836 837 838 839 840 841 845 956 957	1321 1322 1323 1324 1325 1326 1327 1328 1329
958 959 960 961 962 963 964 965 966	1330 1331 1332 1333 1335 1336 1347
967 968 969 970 971 972	

Table 3: Type 5 and 6 of the $C_n^*, n = 13, \ldots, 1612$

n7 430	**n0 IC** 158
18 19 20 21 27 30 35 36 37 39 40 41 42 68 69 70 71 72 73	521 533 536 537 538 541
74 85 102 103 104 106 107 108 109 110 111 112 113 114 115	542 543 546 547 548 864
116 117 118 119 120 169 170 171 172 173 174 175 176 177 178	865 866 867 868 869 870
179 180 181 182 183 184 186 236 237 238 239 240 241 242 244	871 872 873 874 875 876
245 246 247 248 249 250 251 252 253 254 255 256 257 258 259	877 878 879 880 881 882
260 261 262 263 341 342 343 344 345 346 347 348 349 350 351	883 884 885 886 887 888
352 353 354 355 356 357 358 359 360 361 362 363 364 365 366	889 890 891 892 893 894
367 368 372 450 452 453 454 455 456 457 458 459 460 461 462	895 896 897 898 899 900
463 464 465 466 467 468 469 470 471 472 473 474 475 476 477	901 902 903 904 905 906
478 479 480 481 482 483 484 485 500 501 502 605 607 608 609	907 908 909 910 911 912
610 611 613 615 617 618 621 622 625 626 627 628 629 630 631	913 914 915 916 917 918
632 633 635 637 638 639 640 641 642 643 644 645 646 648 754	919 920 921 922 924 925
755 756 757 758 759 760 761 762 774 775 776 815 816 818 819	926 927 928 929 930 931
820 821 822 823 990 991 1024 1026 1206 1207 1208 1209 1210	932 933 934 935 936 937
1211 1221 1222 1223 1224 1225 1226 1227 1228 1229 1230	938 939 940 941 942 943
1231 1232 1233 1234 1235 1236 1237 1238 1239 1240 1241	944 945 946 947 948 949
1242 1243 1244 1245 1246 1247 1248 1249 1250 1251 1252	950 951 952 953 954 955
1253 1254 1255 1256 1257 1258 1259 1260 1261 1262 1263	1367 1368 1369 1370
1264 1265 1266 1267 1268 1269 1270 1271 1272 1273 1274	1371 1372 1373 1374
1275 1276 1277 1278 1279 1280 1281 1282 1283 1284 1285	1375 1376 1377 1378
1286 1287 1288 1289 1290 1291 1292 1293 1294 1295 1296	1379 1380 1381 1382
1297 1298 1299 1300 1301 1302 1303 1304 1305 1306 1307	1383 1384 1385 1386
1308 1309 1310 1311 1312 1313 1314 1334 1337 1338 1339	1387 1388 1389 1390
1340 1341 1342 1343 1344 1345 1346 1348 1349 1350 1351	1391 1392 1393 1394
1352 1353 1354 1355 1356 1357 1358 1359 1360 1361 1362	1395 1396 1397 1398
1363 1364 1365 1366 1423 1424 1425 1426 1427 1428 1429	1399 1400 1401 1402
1430 1431 1432 1433 1434 1435 1436 1437 1438 1439 1440	1403 1404 1405 1406
1441 1442 1443 1444 1445 1446 1447 1448 1449 1450 1451	1407 1408 1409 1410
1452 1453 1454 1455 1456 1457 1458 1459 1460 1461 1462	1411 1412 1413 1414
1463 1464 1465 1466 1467 1468 1469 1470 1471 1472 1473	1415 1416 1417 1418
1474 1475 1476 1477 1478 1479 1480 1481 1482 1483 1484	1419 1420 1421 1422
1485 1486 1487 1488 1489 1490 1491 1492 1493 1494 1495	
1496 1497 1498 1499 1500 1501 1502 1503 1504 1505 1506	
1507 1508 1509 1510 1511 1512 1513 1514 1530	

Table 4: Type 7 and 8 of the $C_n^*, n = 13, \ldots, 1612$

(n, $\mathbf{LJ}_{old}$, $\mathbf{LJ}_{new}$) 65		
(293,-1888.4271,-1888.4274)	(506,-3427.6212,-3427.6875)	(521,-3539.3314,-3539.5098)
(533,-3628.2529,-3629.2999)	(662,-4581.2049,-4581.2058)	(664,-4596.1971,-4596.1978)
(813,-5712.2507,-5712.2517)	(974,-6928.5630,-6928.6305)	(1064,-7616.1673,-7616.1680)
(1075,-7700.8750,-7700.8755)	(1102,-7905.8577,-7905.8651)	(1103,-7913.5579,-7913.5631)
(1106,-7935.9638,-7935.9689)	(1115,-8004.9485,-8004.9868)	(1125,-8081.1711,-8081.1859)
(1126,-8088.8631,-8088.8764)	(1143,-8218.2614,-8218.2690)	(1144,-8225.9422,-8225.9630)
(1146,-8240.8643,-8240.8662)	(1147,-8248.5659,-8248.5706)	(1148,-8256.2554,-8256.2609)
(1158,-8333.0767,-8333.0809)	(1161,-8355.7255,-8355.7298)	(1162,-8363.4124,-8363.4313)
(1163,-8371.1178,-8371.1218)	(1166,-8393.5692,-8393.5838)	(1167,-8401.2616,-8401.2743)
(1179,-8493.0215,-8493.0221)	(1184,-8530.6521,-8530.6600)	(1185,-8538.3320,-8538.3532)
(1187,-8553.2573,-8553.2634)	(1189,-8568.6507,-8568.6566)	(1225,-8844.5625,-8844.5758)
(1243,-8982.2245,-8982.2304)	(1244,-8989.9194,-8989.9244)	(1275,-9229.3690,-9229.3694)
(1287,-9322.0063,-9322.0069)	(1289,-9337.6149,-9337.6157)	(1292,-9360.2960,-9360.2969)
(1294,-9375.7081,-9375.7091)	(1312,-9515.0285,-9515.0327)	(1315,-9537.6838,-9537.6880)
(1317,-9553.0747,-9553.0788)	(1324,-9606.7794,-9606.7798)	(1336,-9699.4110,-9699.4116)
(1338,-9715.0285,-9715.0314)	(1341,-9737.7061,-9737.7094)	(1343,-9753.1169,-9753.1200)
(1366,-9930.4757,-9930.4764)	(1445,-10538.9878,-10538.9883)	
(1457,-10631.4452,-10631.4458)	(1483,-10831.4787,-10831.4791)	
(1488,-10869.6845,-10869.6917)	(1489,-10877.3862,-10877.4015)	
(1490,-10885.0944,-10885.1024)	(1523,-11139.7180,-11139.7228)	
(1526,-11162.5614,-11162.5647)	(1528,-11178.2283,-11178.2291)	
(1552,-11364.4027,-11364.4088)	(1554,-11380.0717,-11380.0735)	
(1558,-11410.7180,-11410.7193)	(1585,-11620.2304,-11620.2305)	
(1595,-11698.0815,-11698.0820)	(1611,0.0000,-11821.7581)	(1612,0.0000,-11829.4494)

Table 5: New C_n^*

[7] S. Gómez and C. Barrón-Romero. The Exponential Tunneling Method. Technical Report Research Report 3(1), IIMAS-UNAM, Julio 1991 1991.

[8] M. R. Hoare and J. A. McInnes. Morphology and statistical statics of simple microclusters. *Advances in Physics*, 32(5):791–821, 1983.

[9] M. R. Hoare and P. Pal. Physical cluster mechanics: statistical thermodynamics and nucleation theory for monatomic systems. *Advances in Physics*, 24(5):645–678, 1975.

[10] R. H. Leary. Global Optima of Lennard-Jones Clusters. *Journal of Global Optimization*, 11(1):35–53, 1997.

[11] R. Maier, J. Rosen, and G. Xue. A discrete-continuous algorithm for molecular energy minimization. In *Proceedings. Supercomputing '92. (Cat. No.92CH3216-9), 16-20 Nov. 1992*, Proceedings. Supercomputing '92. (Cat. No.92CH3216-9), pages 778–786, Minneapolis, MN, USA, 1992. IEEE Comput. Soc. Press.

[12] J. A. Northby. Structure and binding of Lennard-Jones clusters: $13 \leq n \leq 147$. *Journal of Chemical Physics*, 87(10):6166–6177, 1987.

[13] D. Romero, C. Barrón-Romero, and S. Gómez. The optimal configurations of LJ atomic clusters: 148-309. In *Siam Annual Meeting*, Atlanta, GA, USA, 1999.

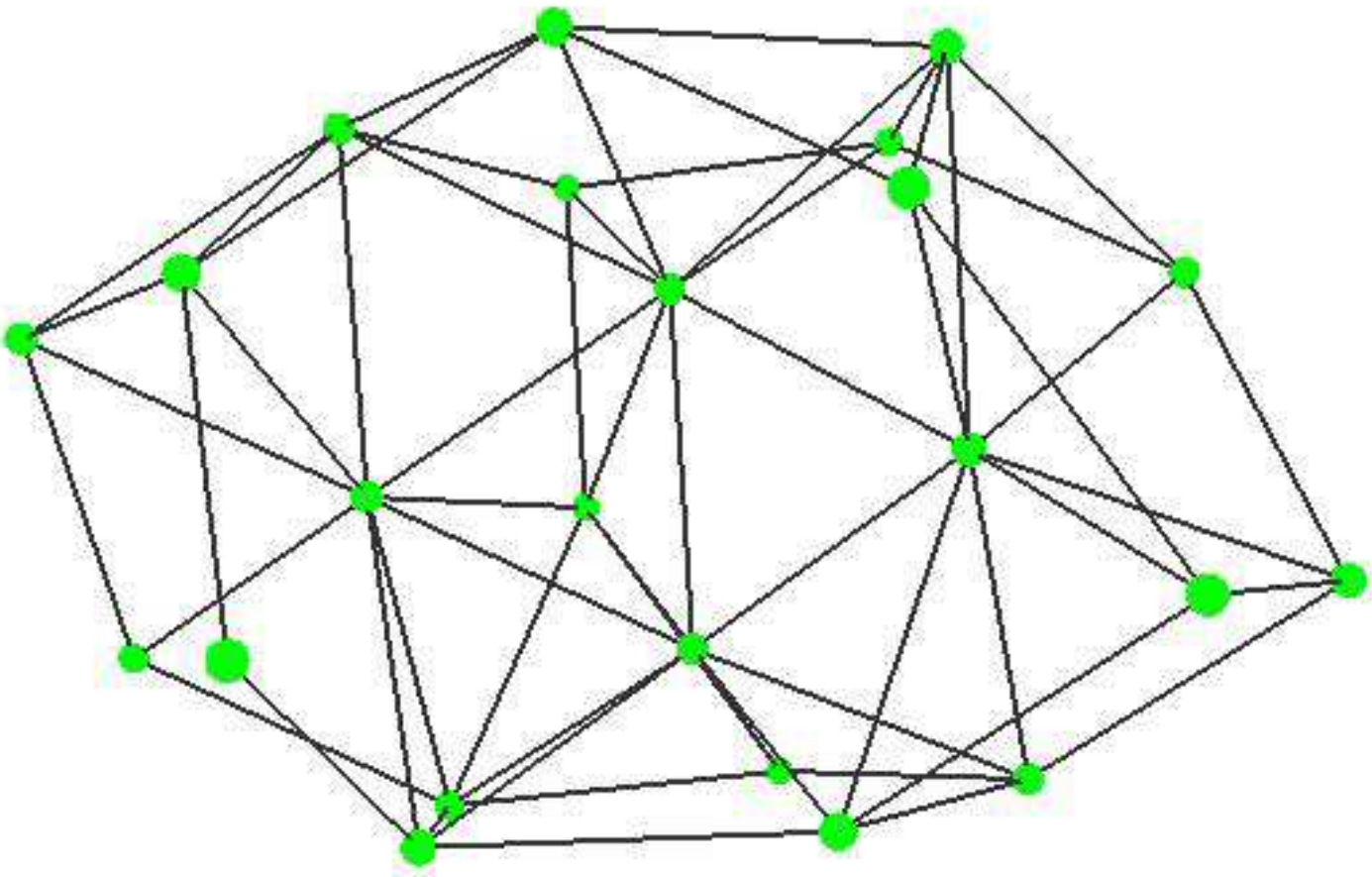
[14] D. Romero, C. Barrón-Romero, and S. Gómez. The optimal geometry of Lennard-Jones clusters: 148-309. *Computer Physics Communications*, 123:87–96, 1999.

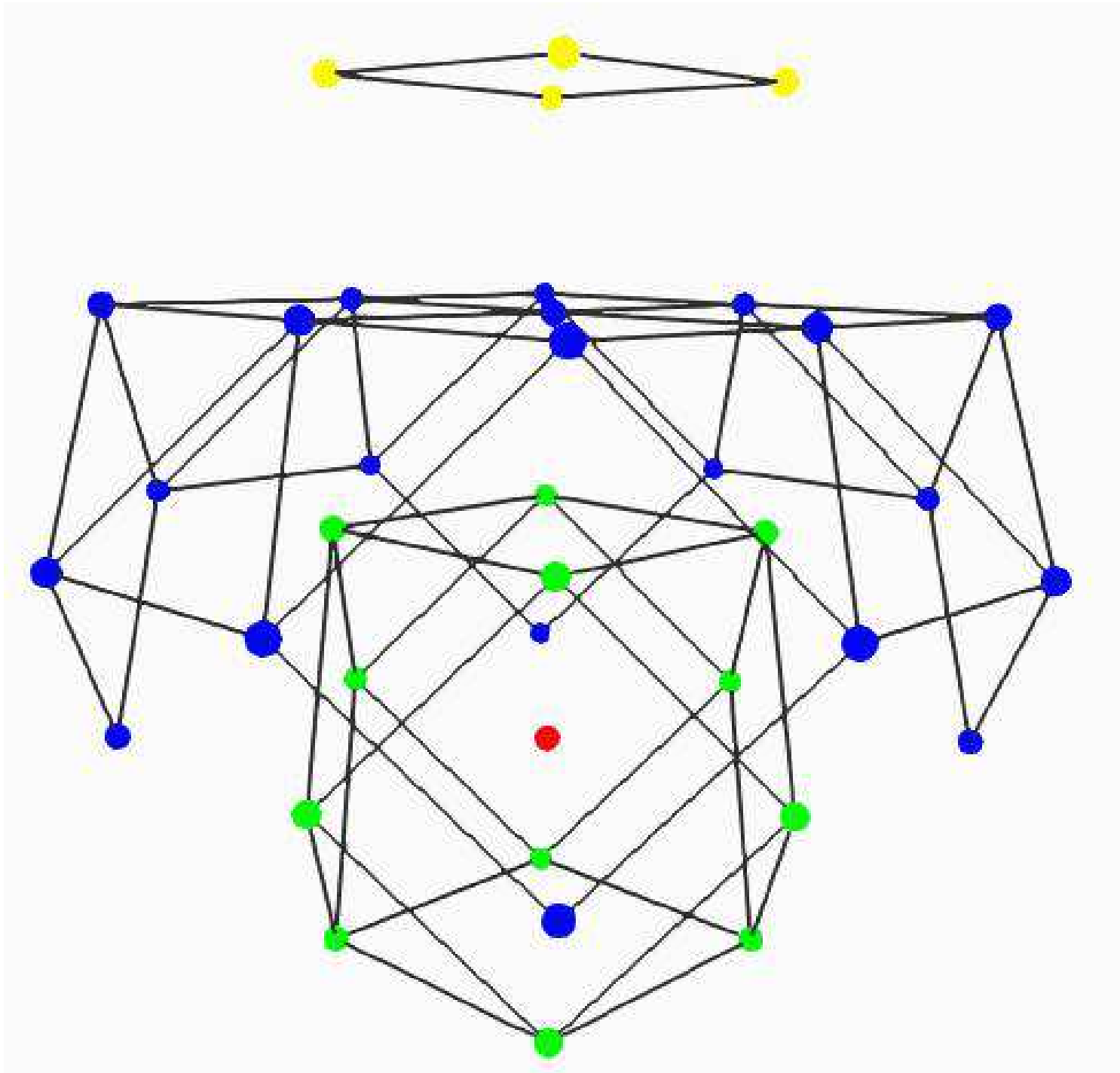
[15] X. Shao, Y. Xiang, and W. Cai. Structural Transition from Icosahedra to Decahedra of Large Lennard-Jones Clusters. *Personal Communication*, 2005.

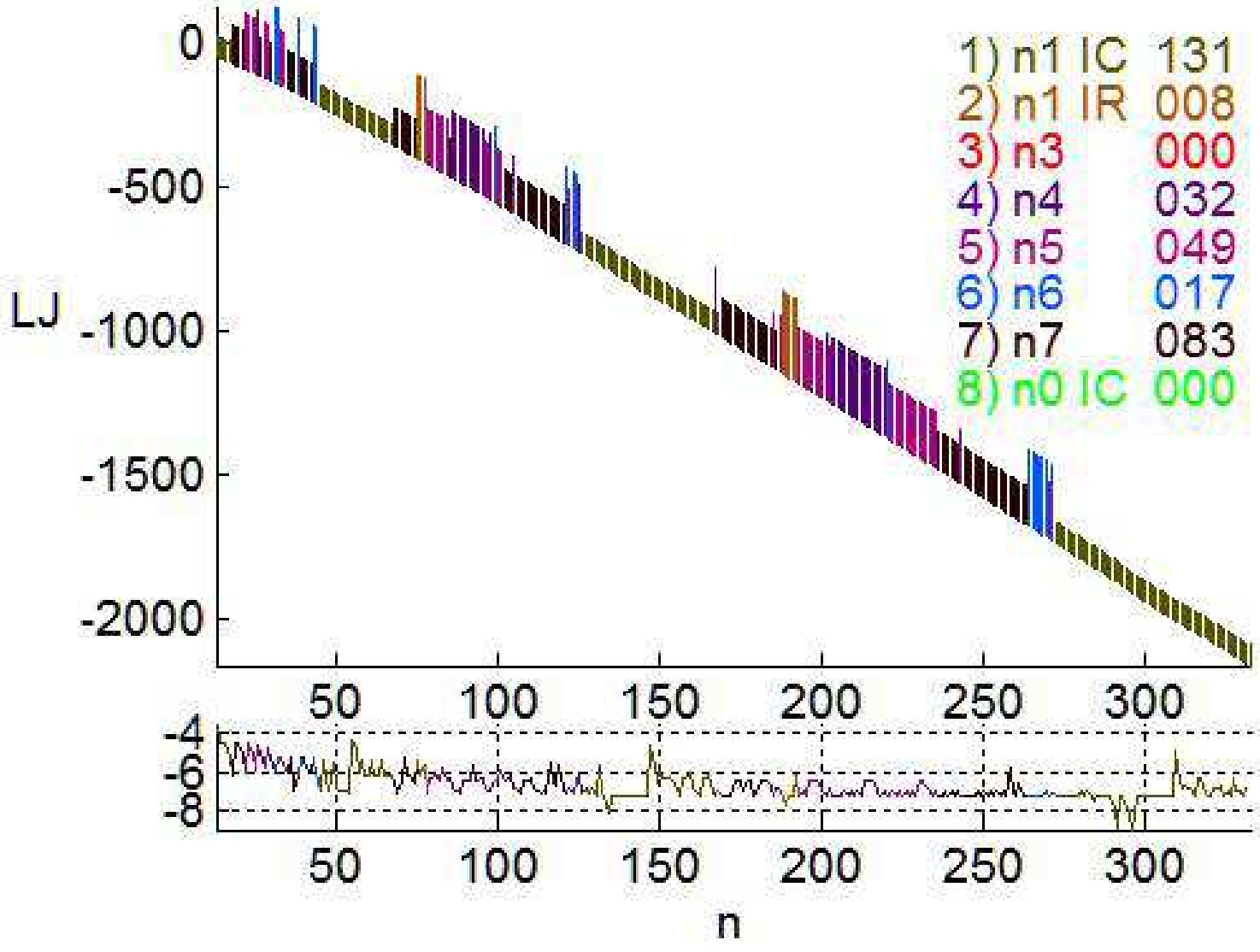
[16] I. A. Solov'yov, A. V. Solov'yov, and W. Greiner. Fusion process of Lennard-Jones clusters: global minima and magic numbers formation. *ArXiv Physics e-prints*, pages 1–47, 2003.

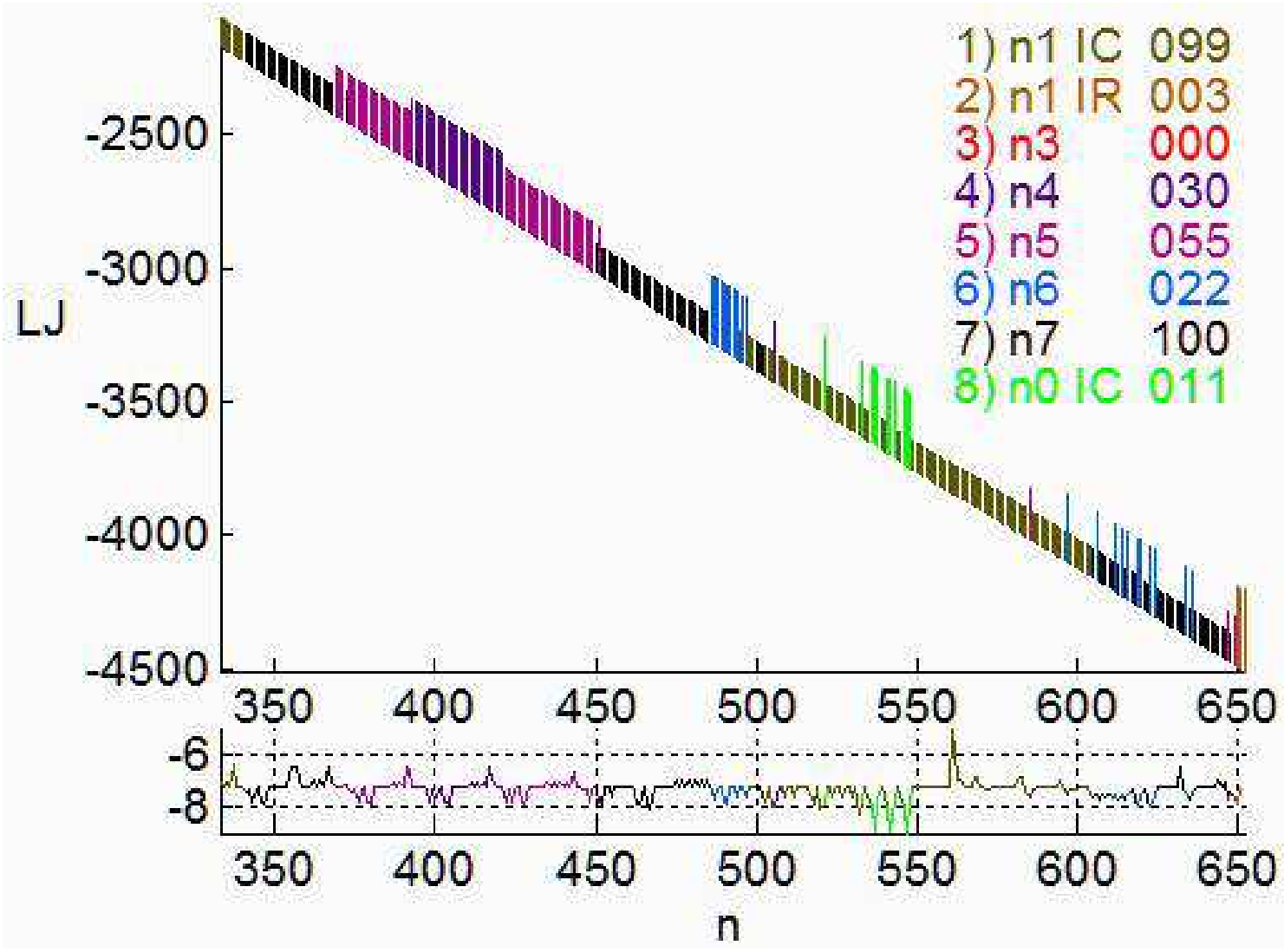
[17] D. J. Wales, J. P. K. Doye, A. Dullweber, M. P. Hodges, F. Y. Naumkin, F. Calvo, J. Hernández-Rojas, and T. F. Middleton. The cambridge cluster database, lennard-jones clusters, http://www-doye.ch.cam.ac.uk/jon/structures/lj.html.

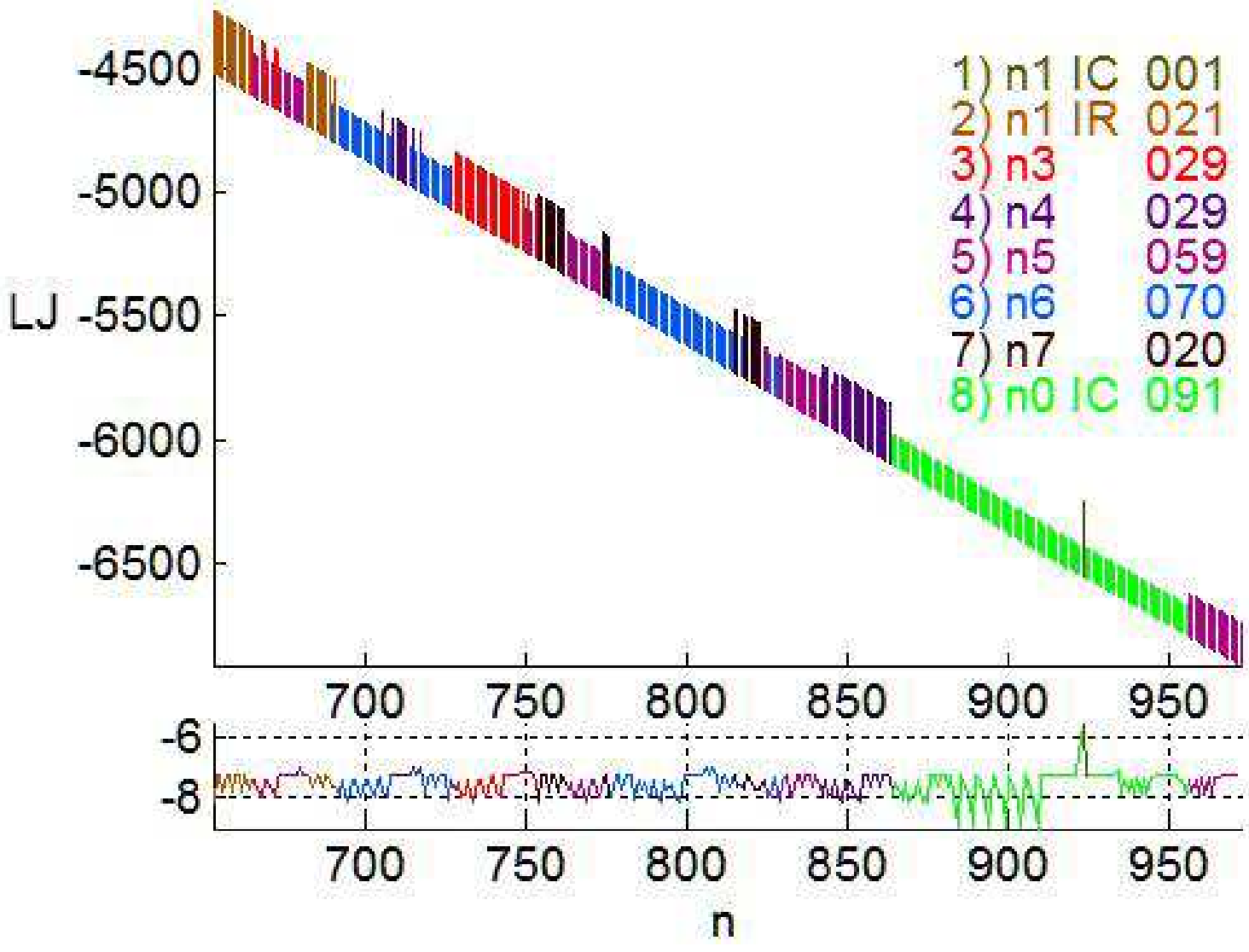
[18] Y. Xiang, H. Jiang, W. Cai, and X. Shao. An Efficient Method Based on Lattice Construction and the Genetic Algorithm for Optimization of Large Lennard-Jones Clusters. *Journal of Physical Chemistry A*, 108(16):3586–92, 2004.

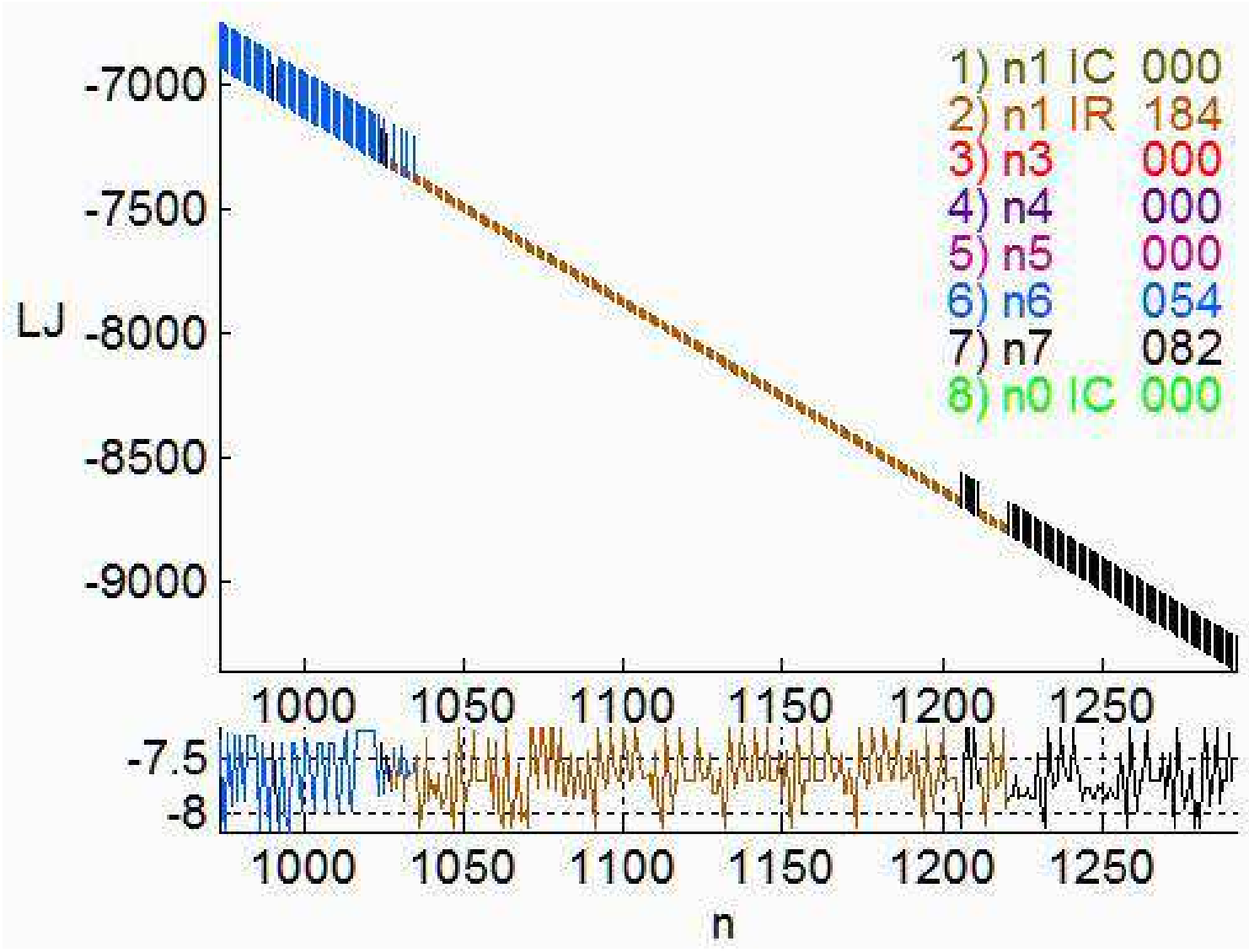


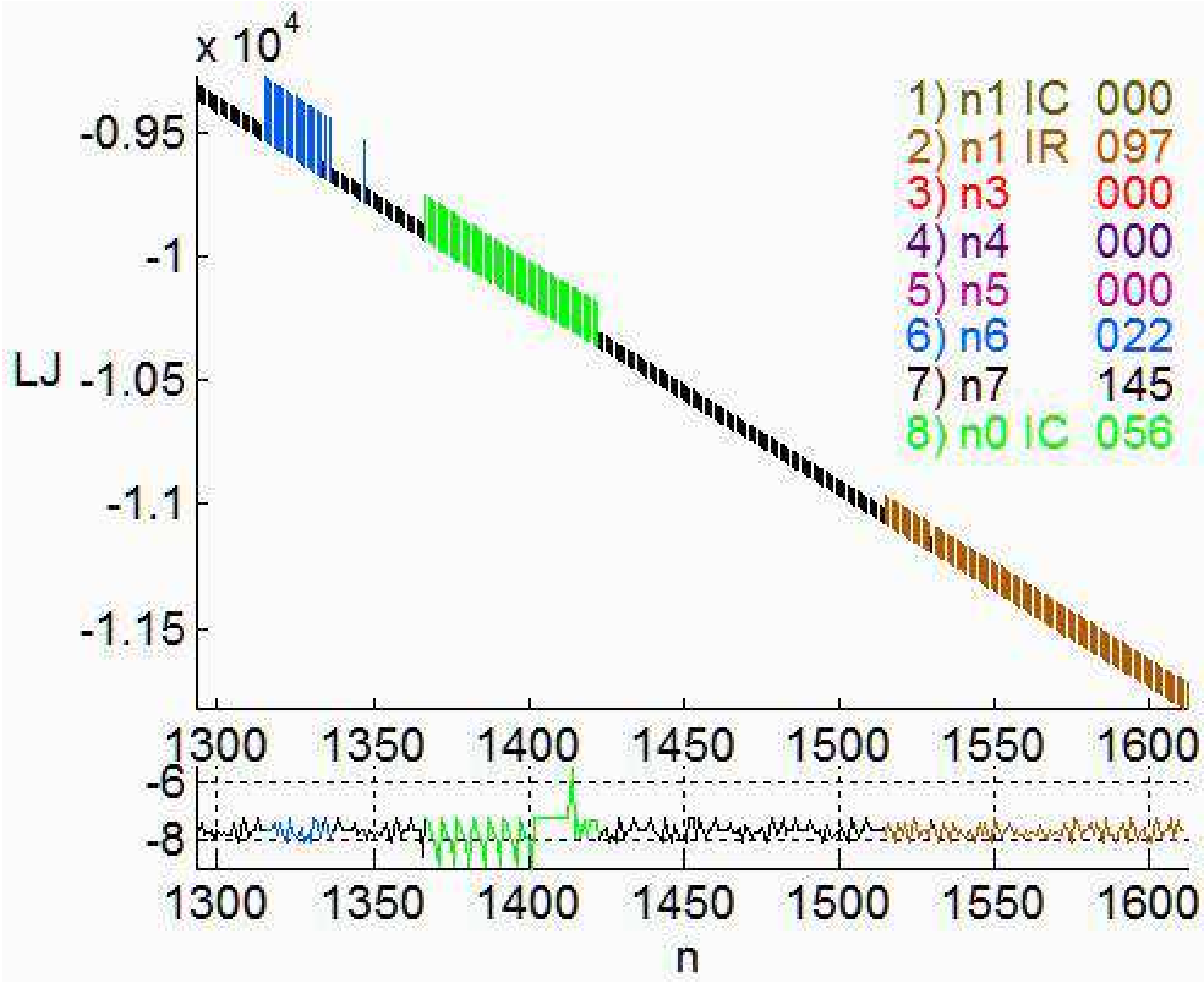


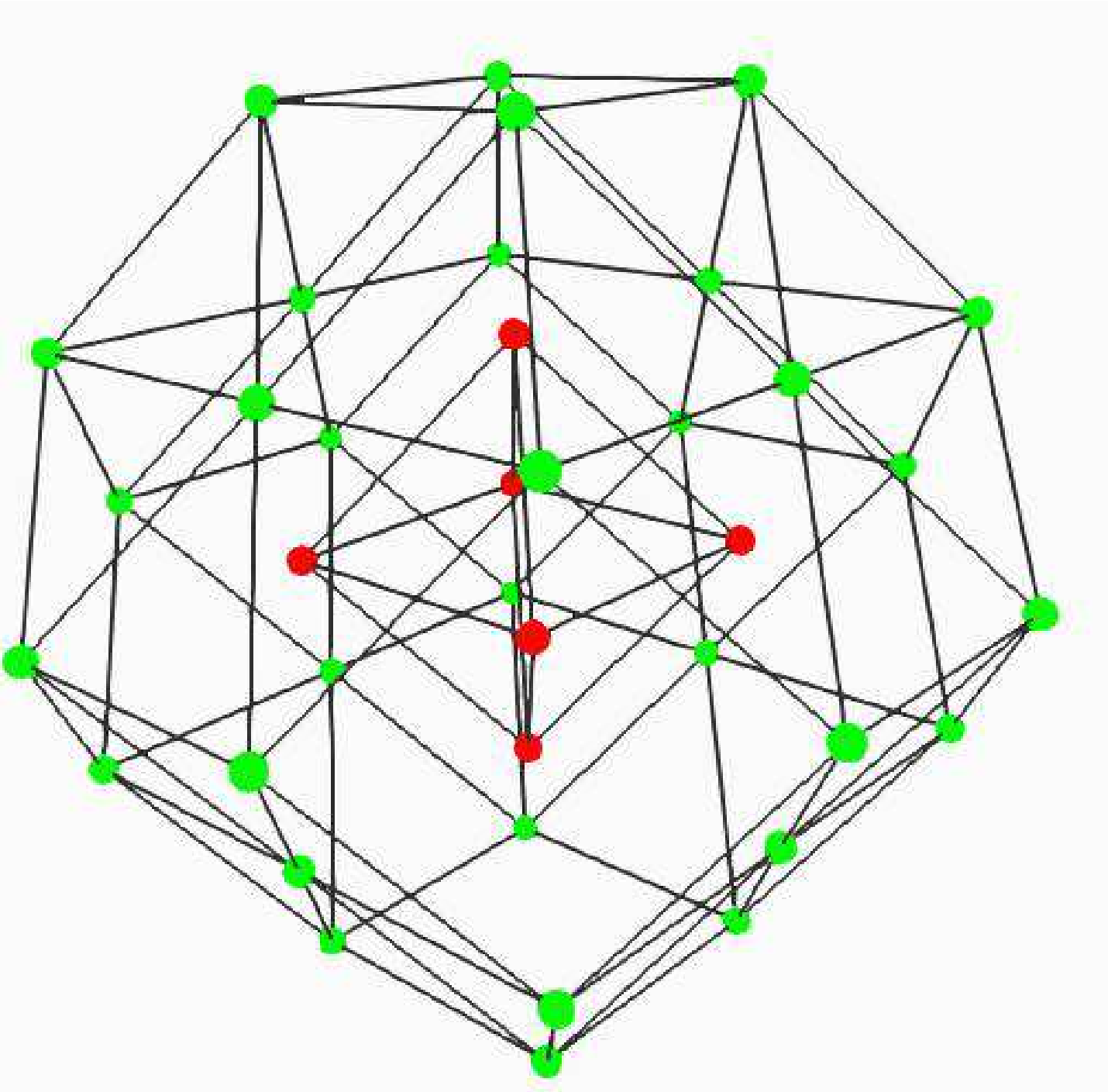

0
-500
-1000
-1500
-2000
LJ
1) n1 IC 131
2) n1 IR 008
3) n3 000
4) n4 032
5) n5 049
6) n6 017
7) n7 083
8) n0 IC 000
50
100
150
200
250
300
-4
-6
-8
n

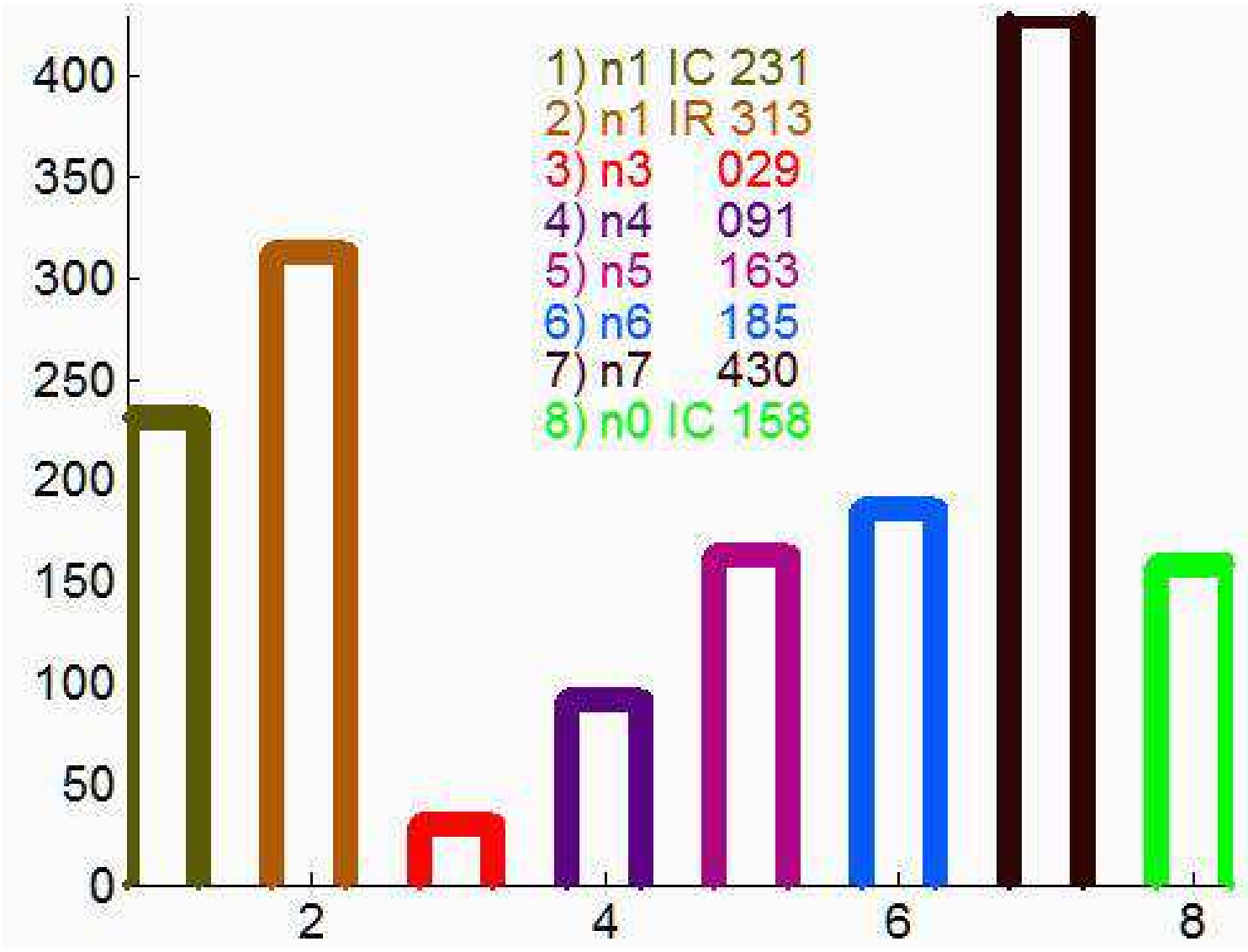

1) n1 IC 099
2) n1 IR 003
3) n3 000
4) n4 030
5) n5 055
6) n6 022
7) n7 100
8) n0 IC 011
LJ
-2500
-3000
-3500
-4000
-4500
350
400
450
500
550
600
650
-6
-8
n

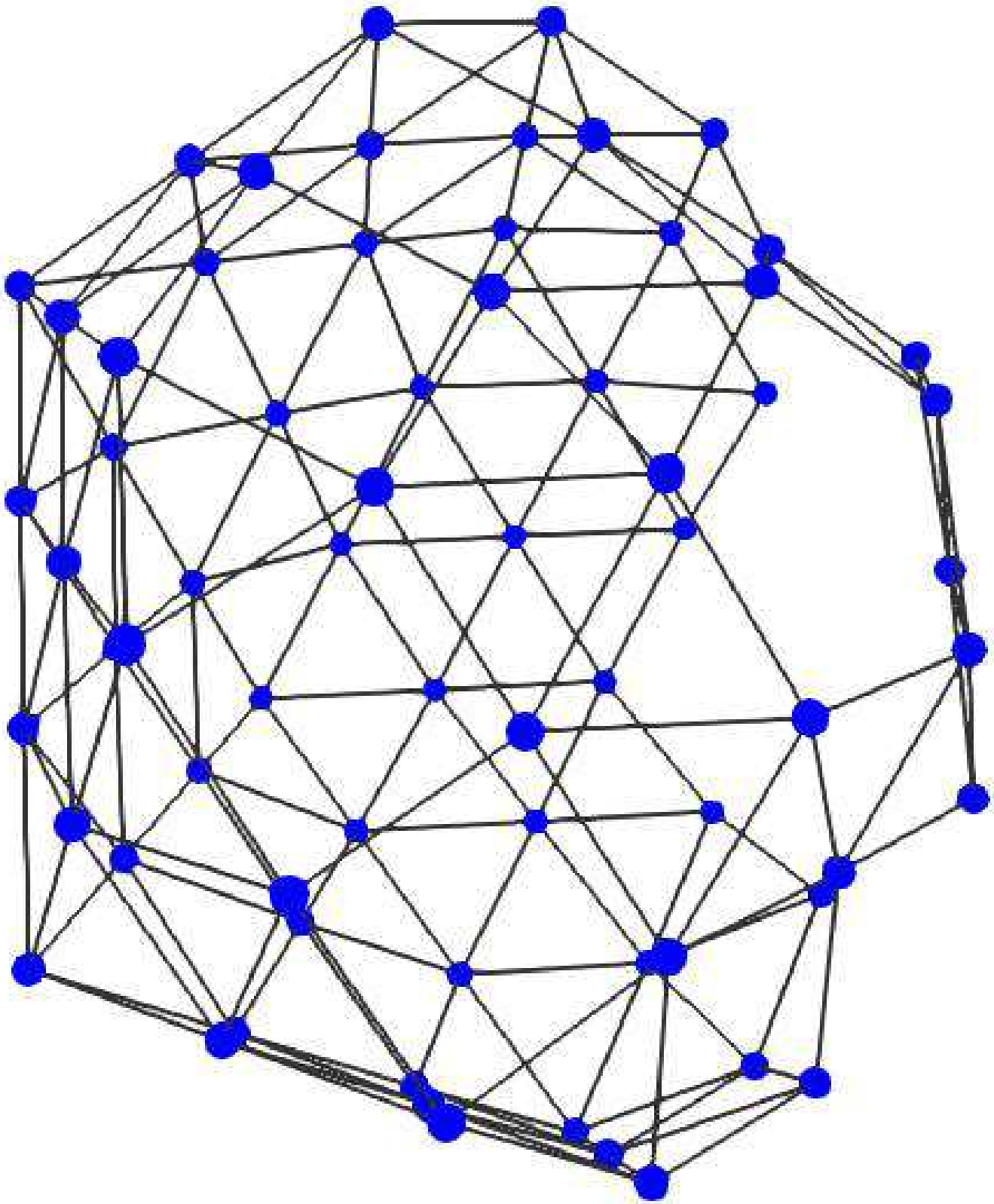

-4500
-5000
LJ -5500
-6000
-6500
1) n1 IC 001
2) n1 IR 021
3) n3 029
4) n4 029
5) n5 059
6) n6 070
7) n7 020
8) n0 IC 091
700
750
800
850
900
950
-6
-8
700
750
800
850
900
950
n

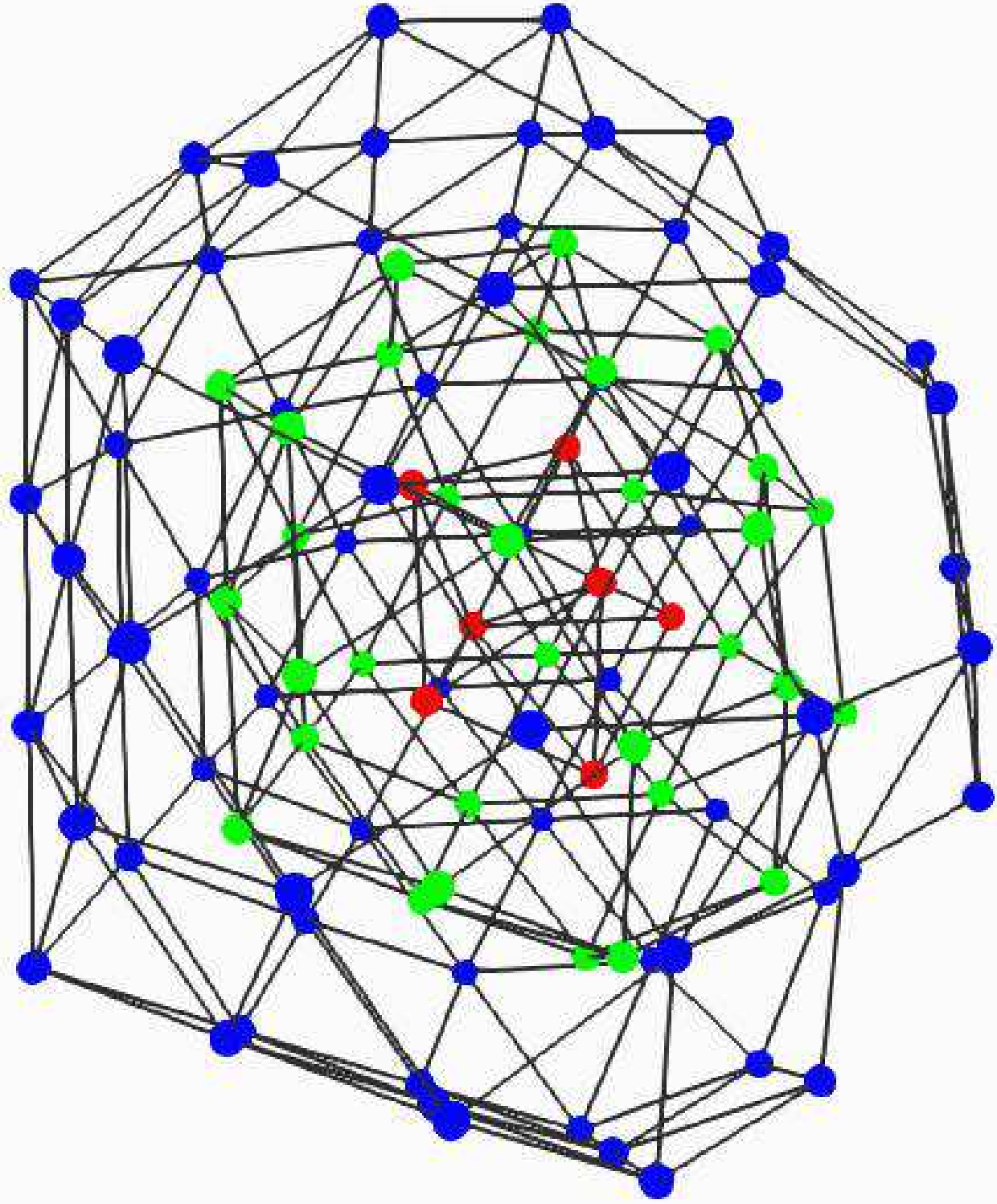

1) n1 IC 000
2) n1 IR 184
3) n3 000
4) n4 000
5) n5 000
6) n6 054
7) n7 082
8) n0 IC 000
LJ
-7000
-7500
-8000
-8500
-9000
1000
1050
1100
1150
1200
1250
-7.5
-8
n

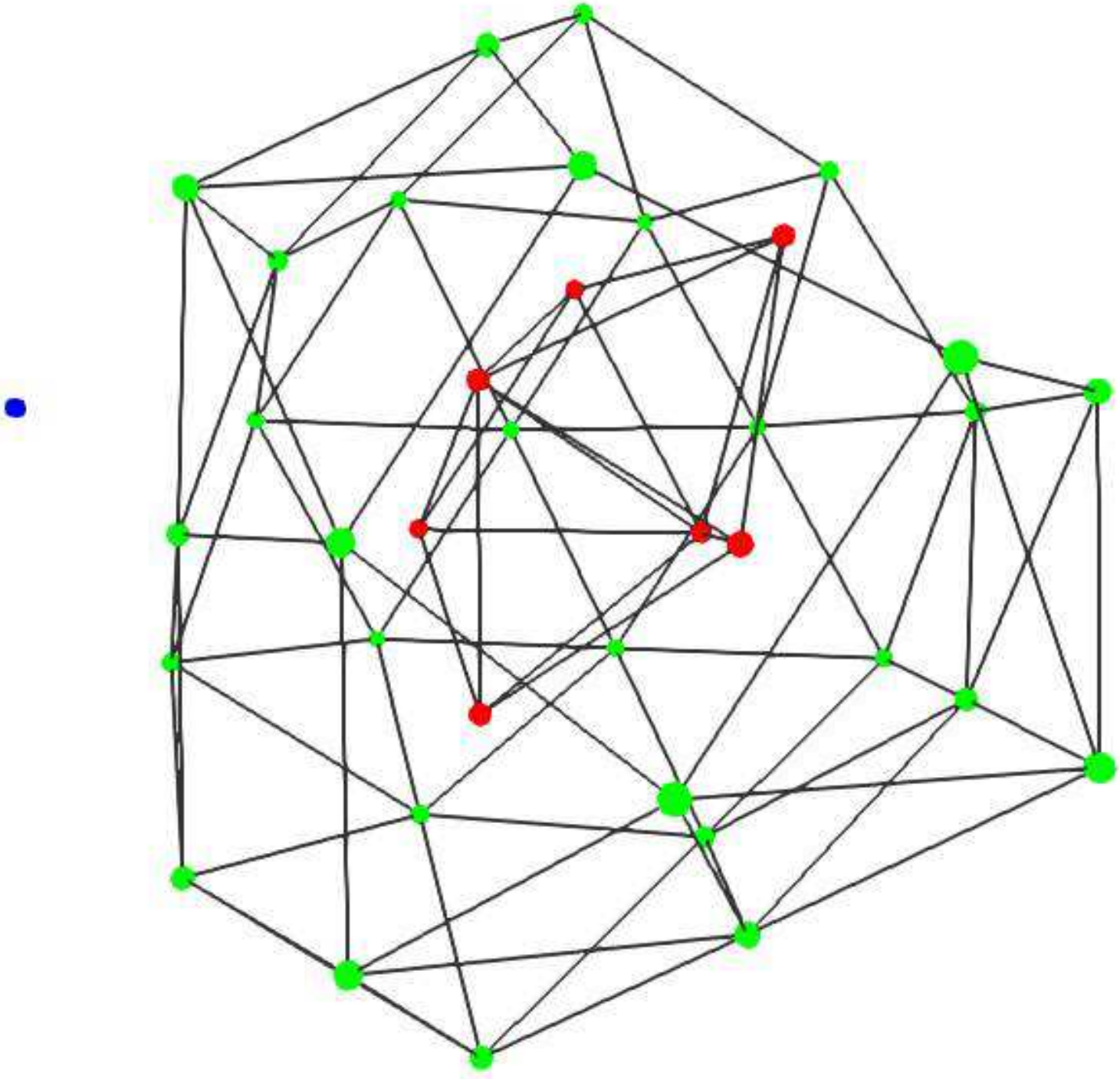

x 10^4
-0.95
-1
-1.05
-1.1
-1.15
LJ
1) n1 IC 000
2) n1 IR 097
3) n3 000
4) n4 000
5) n5 000
6) n6 022
7) n7 145
8) n0 IC 056
1300
1350
1400
1450
1500
1550
1600
-6
-8
n

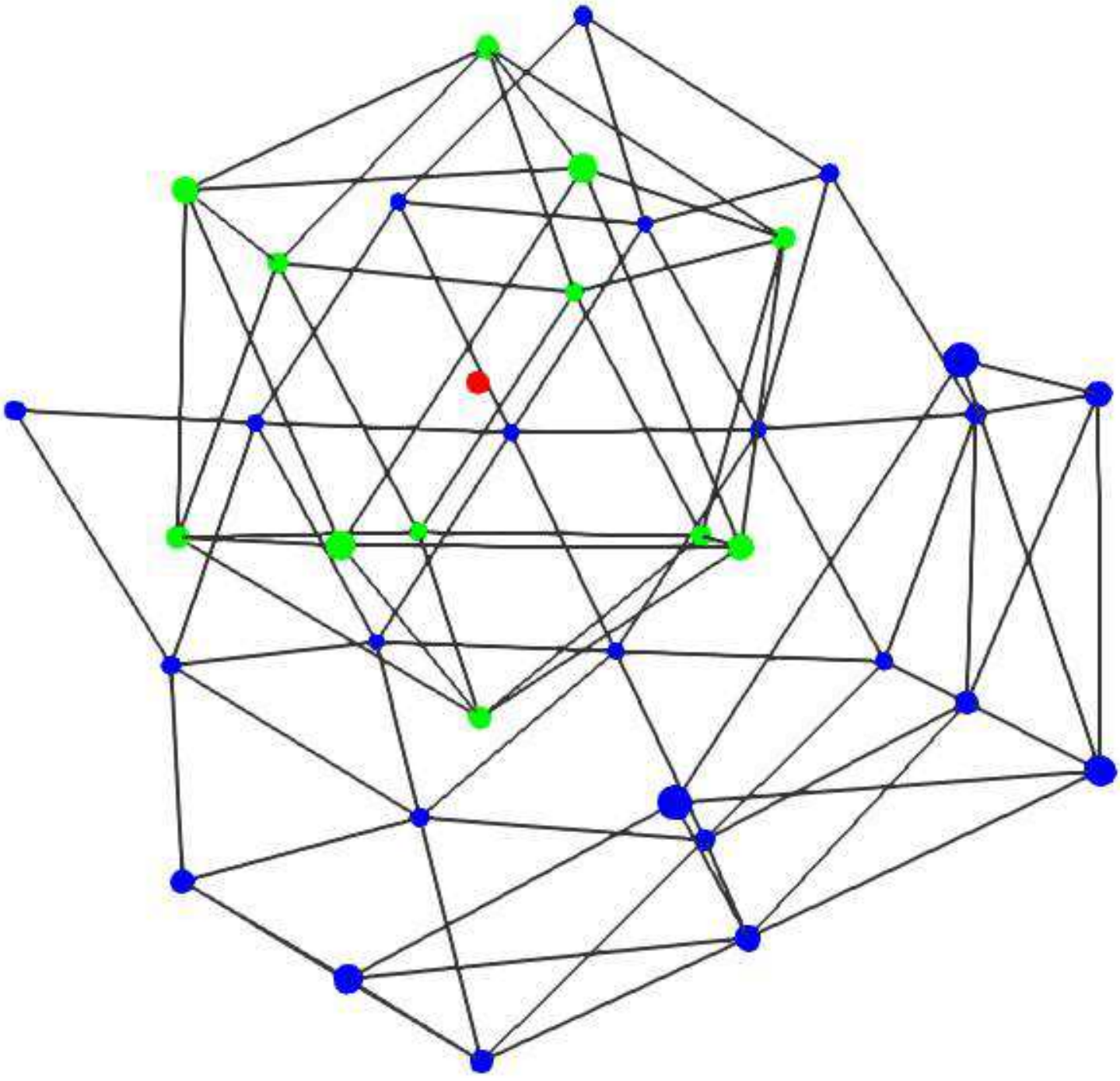


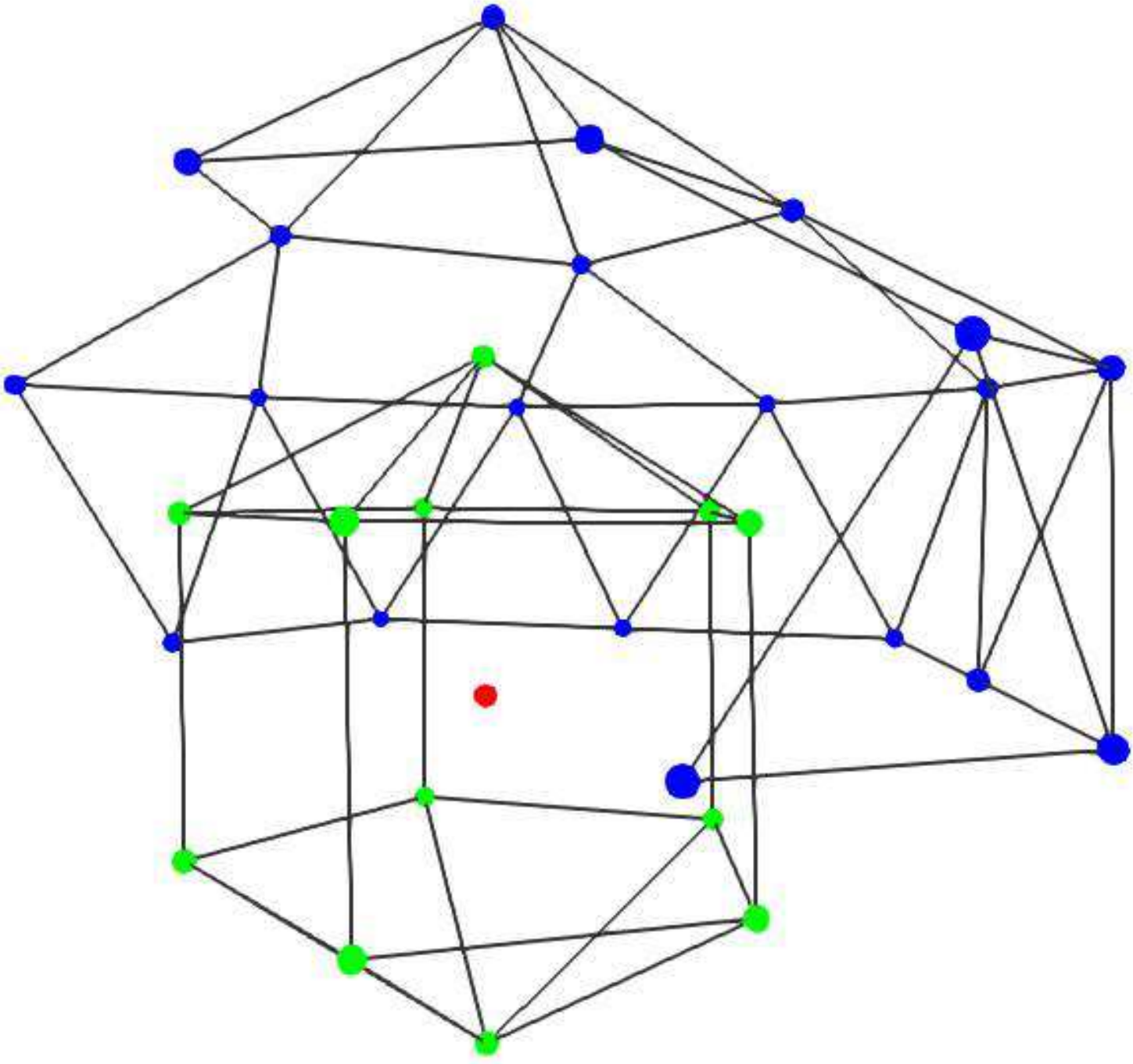

1) n1 IC 231
2) n1 IR 313
3) n3 029
4) n4 091
5) n5 163
6) n6 185
7) n7 430
8) n0 IC 158
400
350
300
250
200
150
100
50
0
2
4
6
8

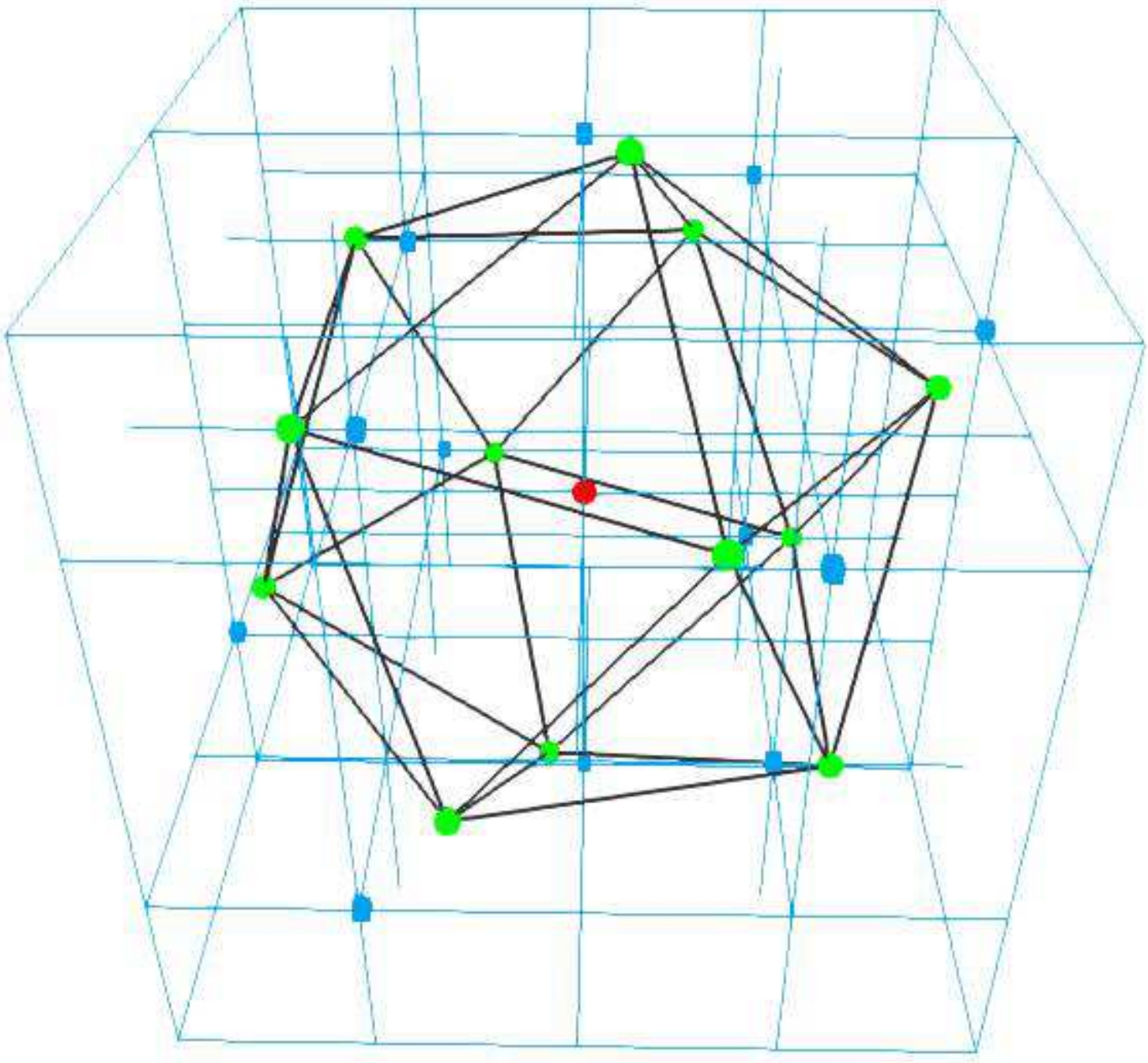


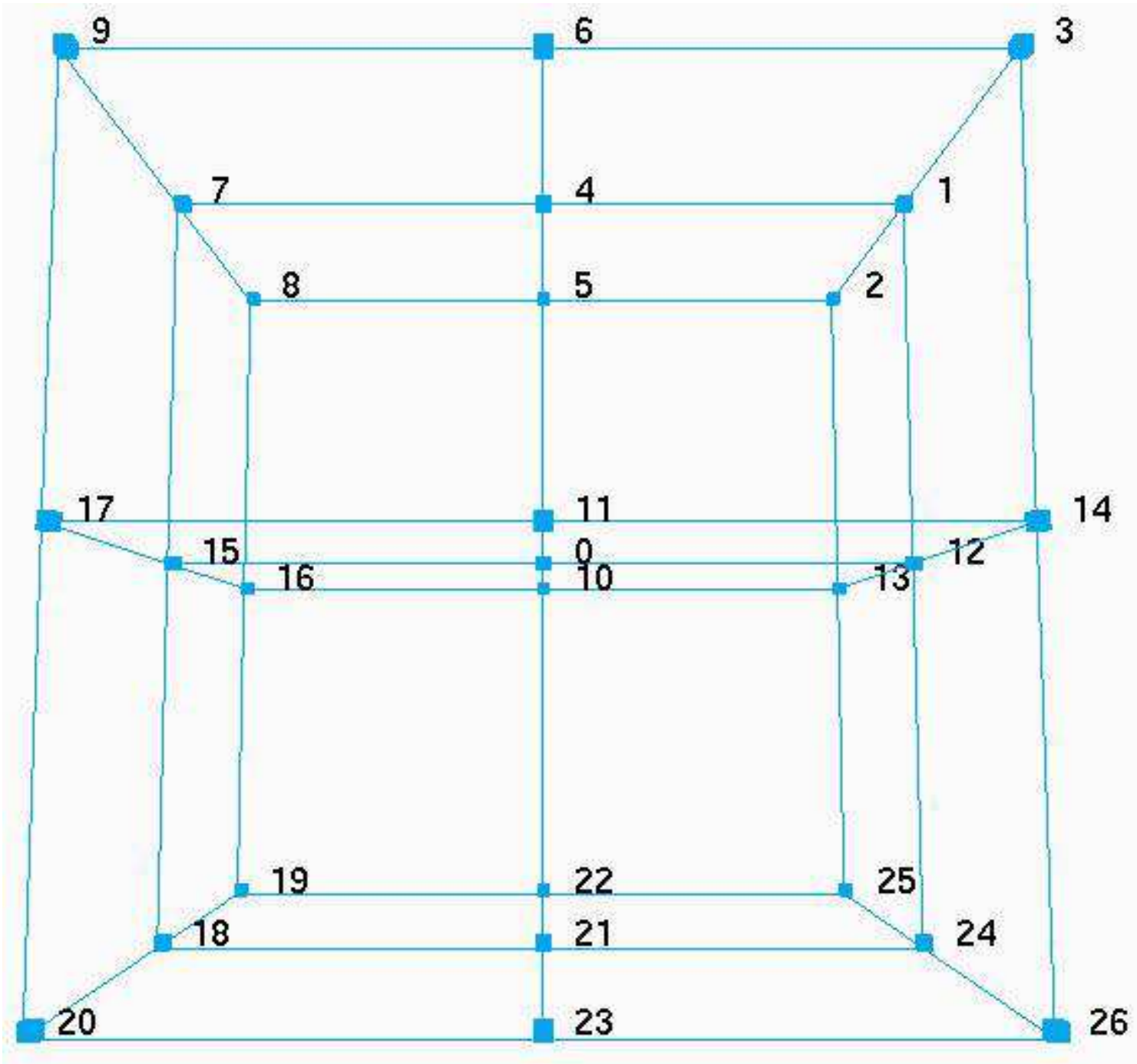


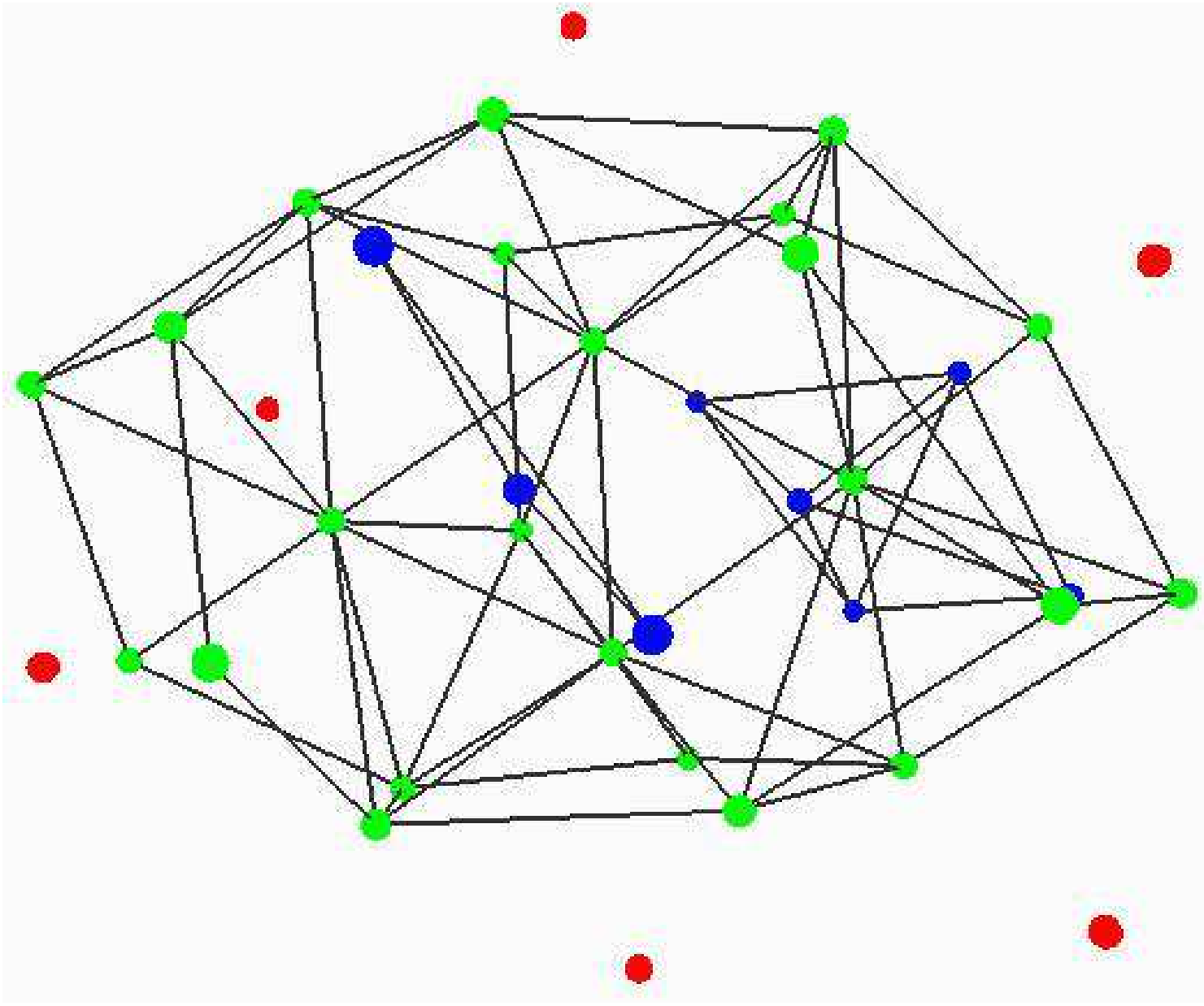


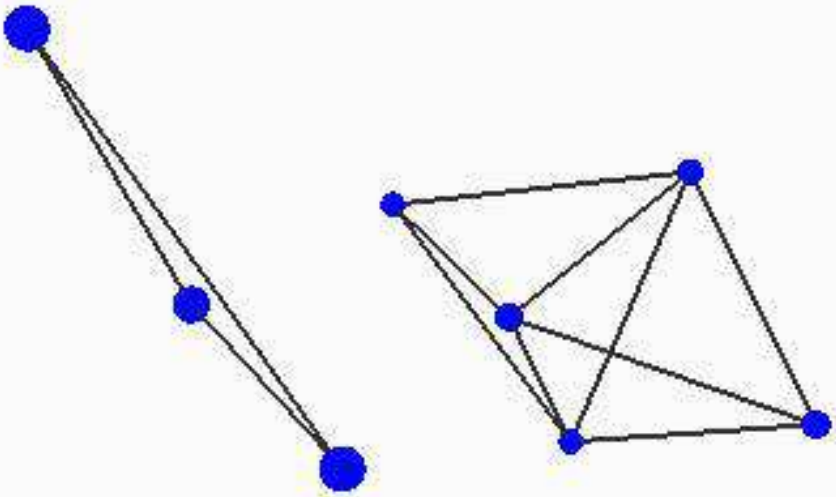


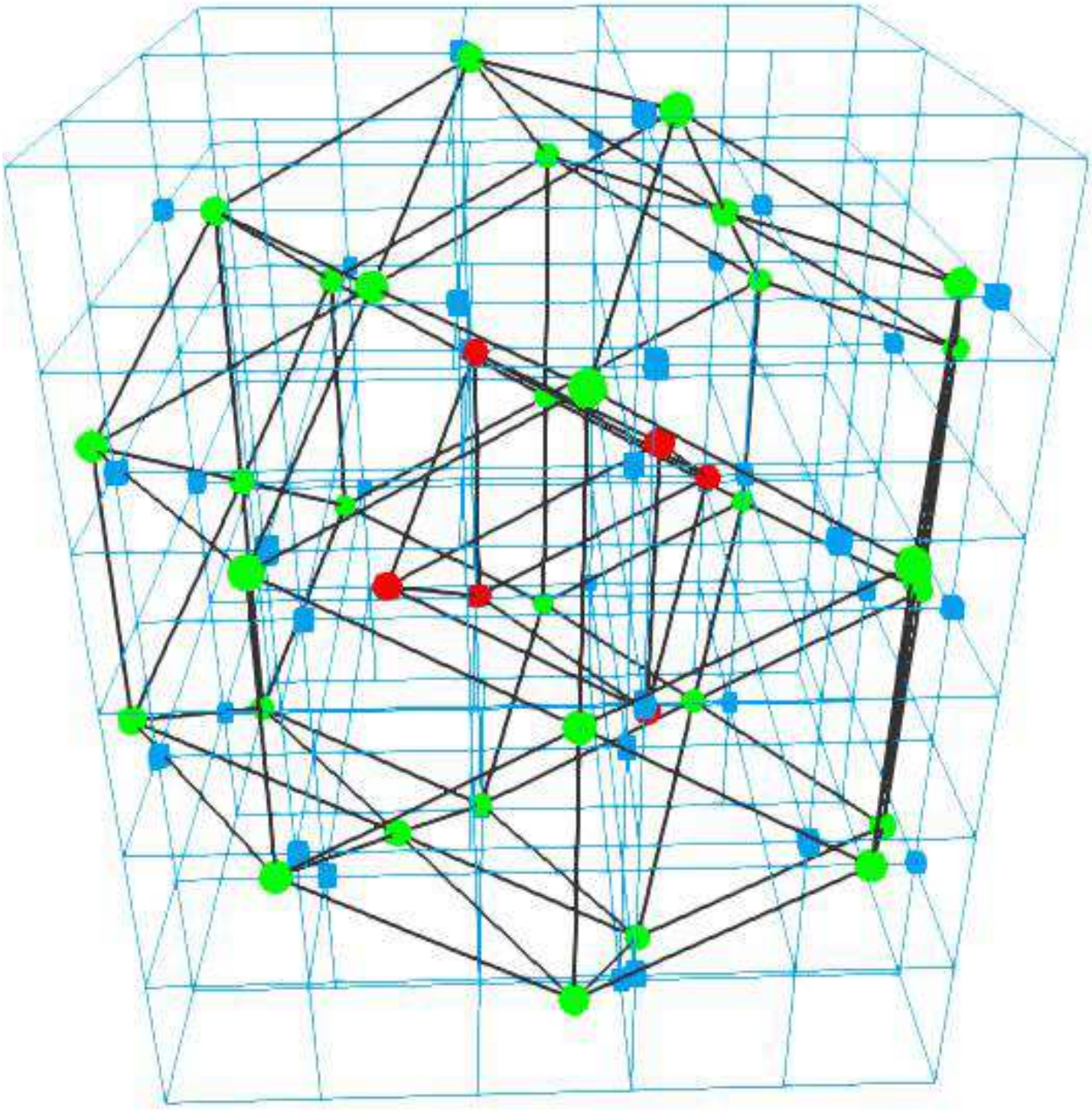


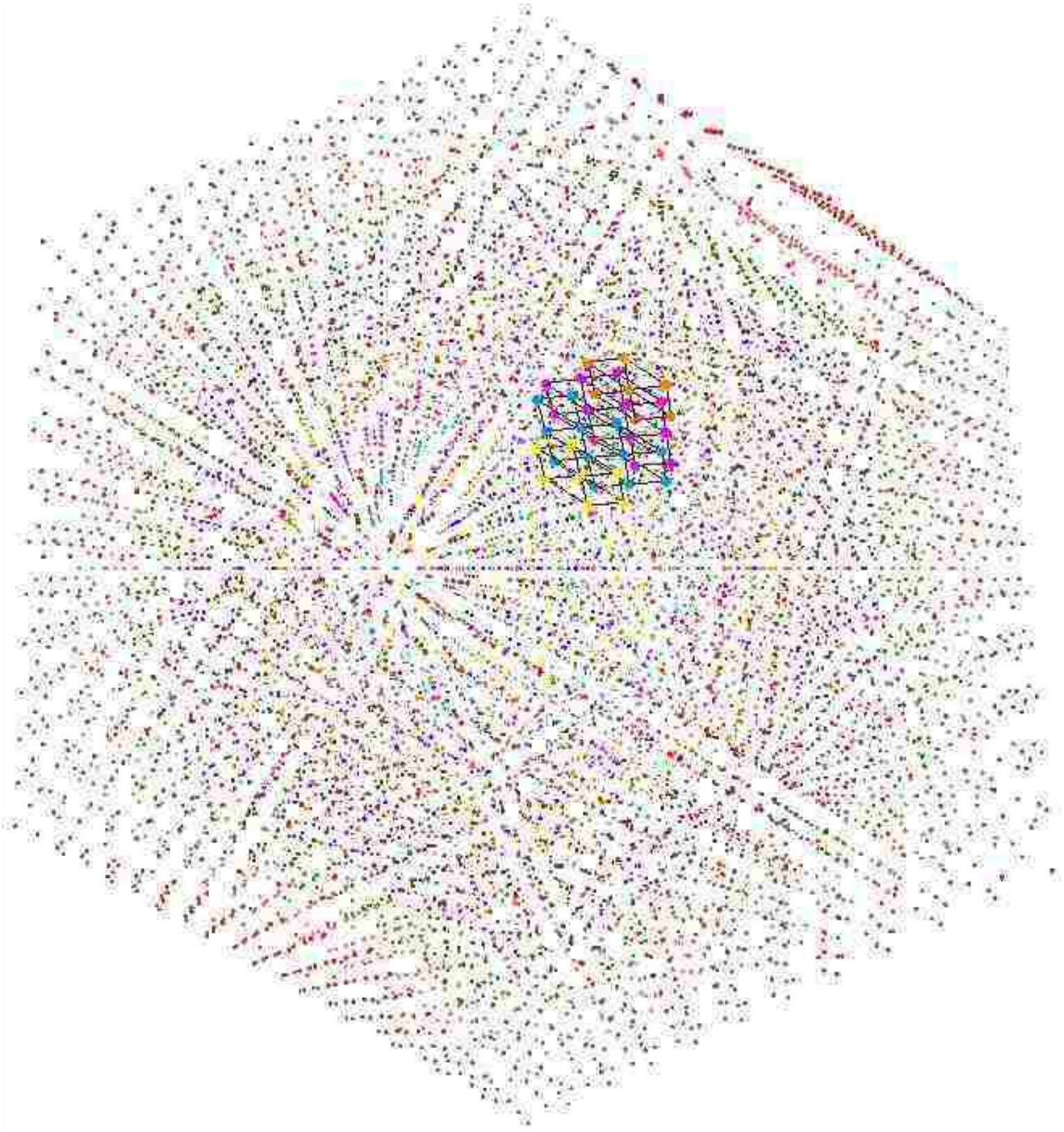


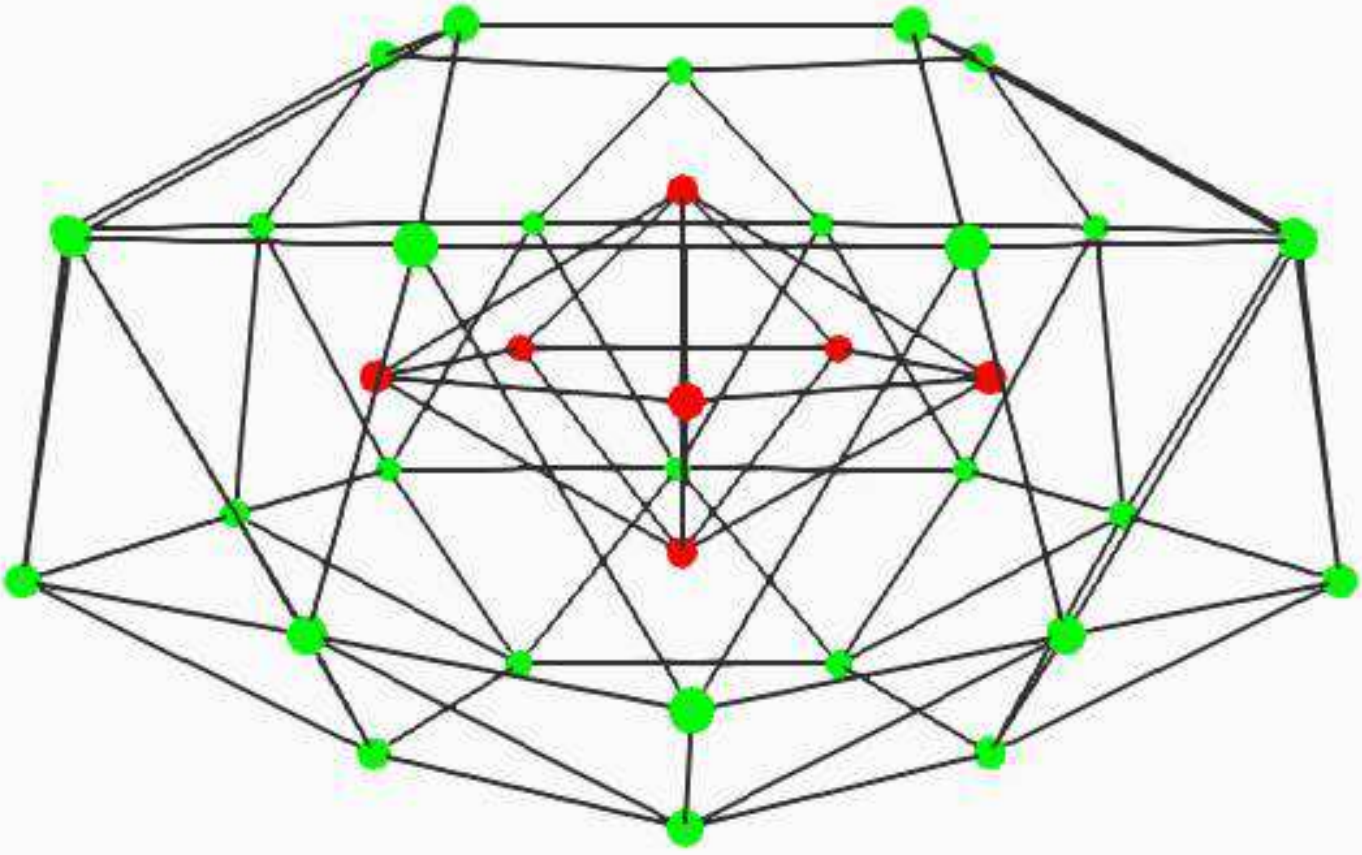

9
6
3
7
4
1
8
5
2
17
11
14
15
0
12
16
10
13
19
22
25
18
21
24
20
23
26

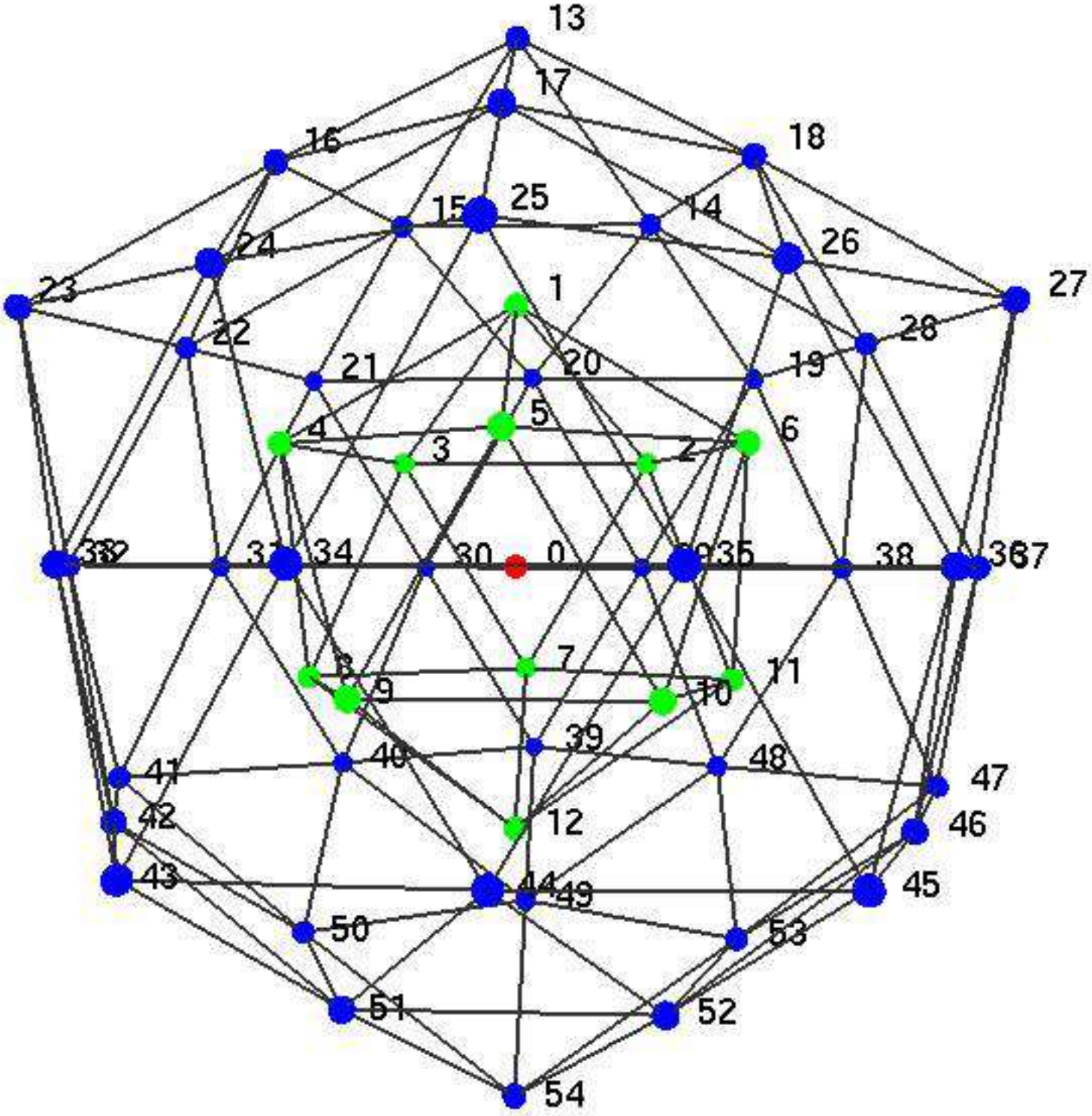











13
17
16
18
15
25
14
24
26
23
27
1
22
28
21
20
19
5
4
6
3
2
0
34
30
38
7
9
10
11
39
40
48
41
47
42
12
46
43
44
49
45
50
53
51
52
54