The study of energy states in the Thomson problem

Stepan Fadeev
Novosibirsk State University
stepan-fadeev@mail.ru
Vasily Dedok
Sobolev Institute of Mathematics, Novosibirsk, Russia
dedok@math.nsc.ru

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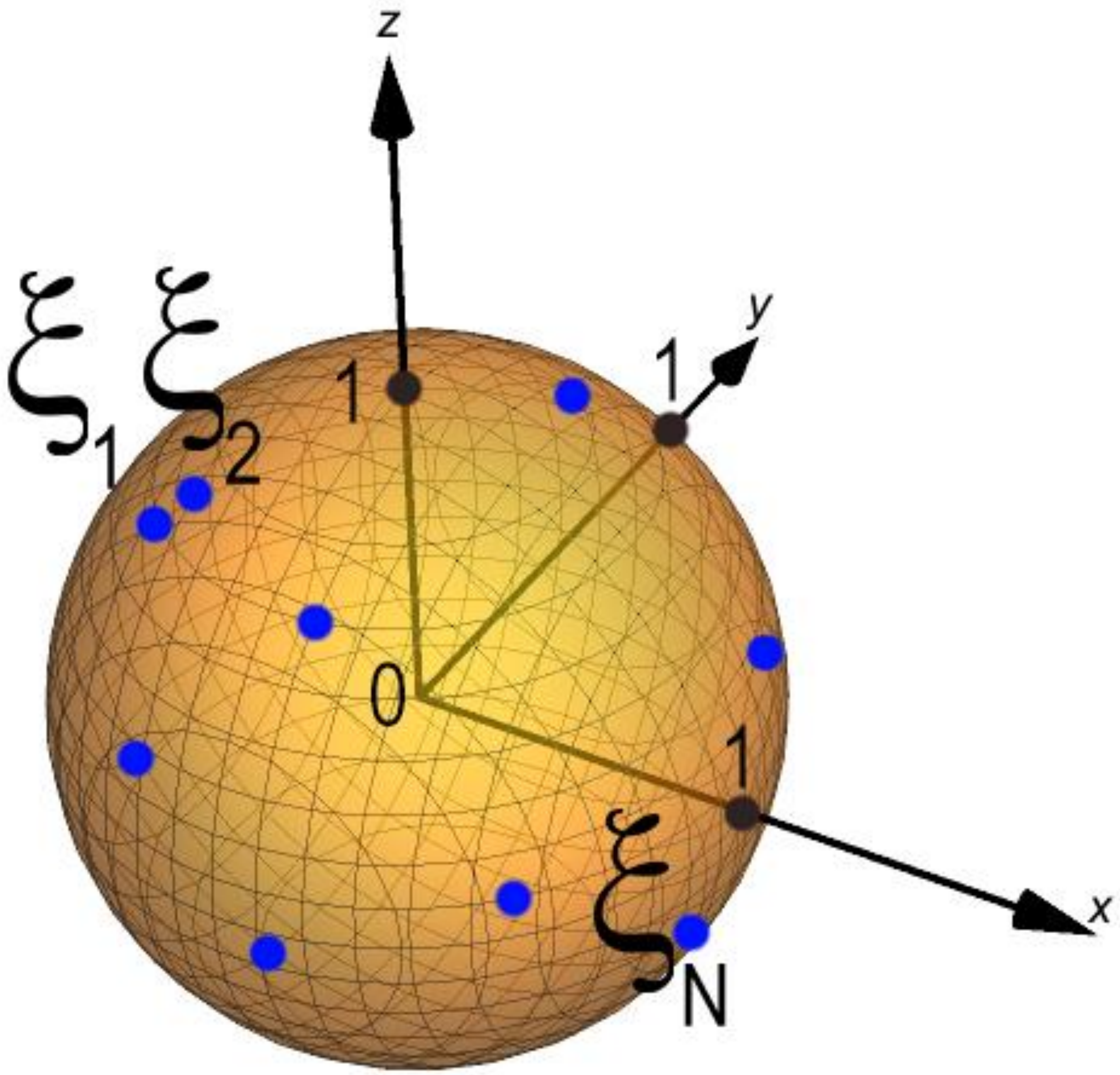
Presentation plan

- Introduction
- Methods for solving the Thomson problem
- A direct algorithm for verifying graph isomorphism
- Results of numerical simulation
- Conclusion

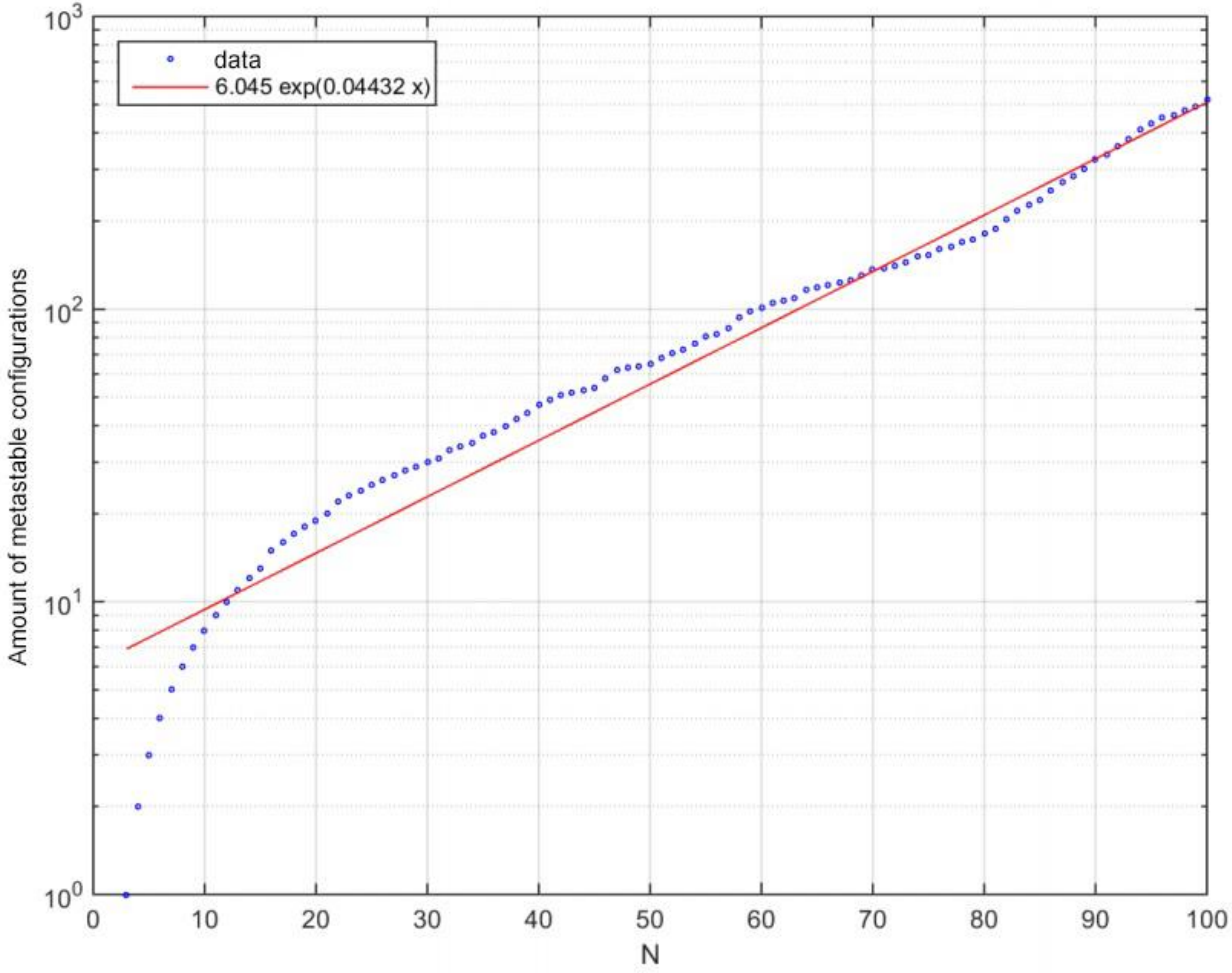
Thomson problem



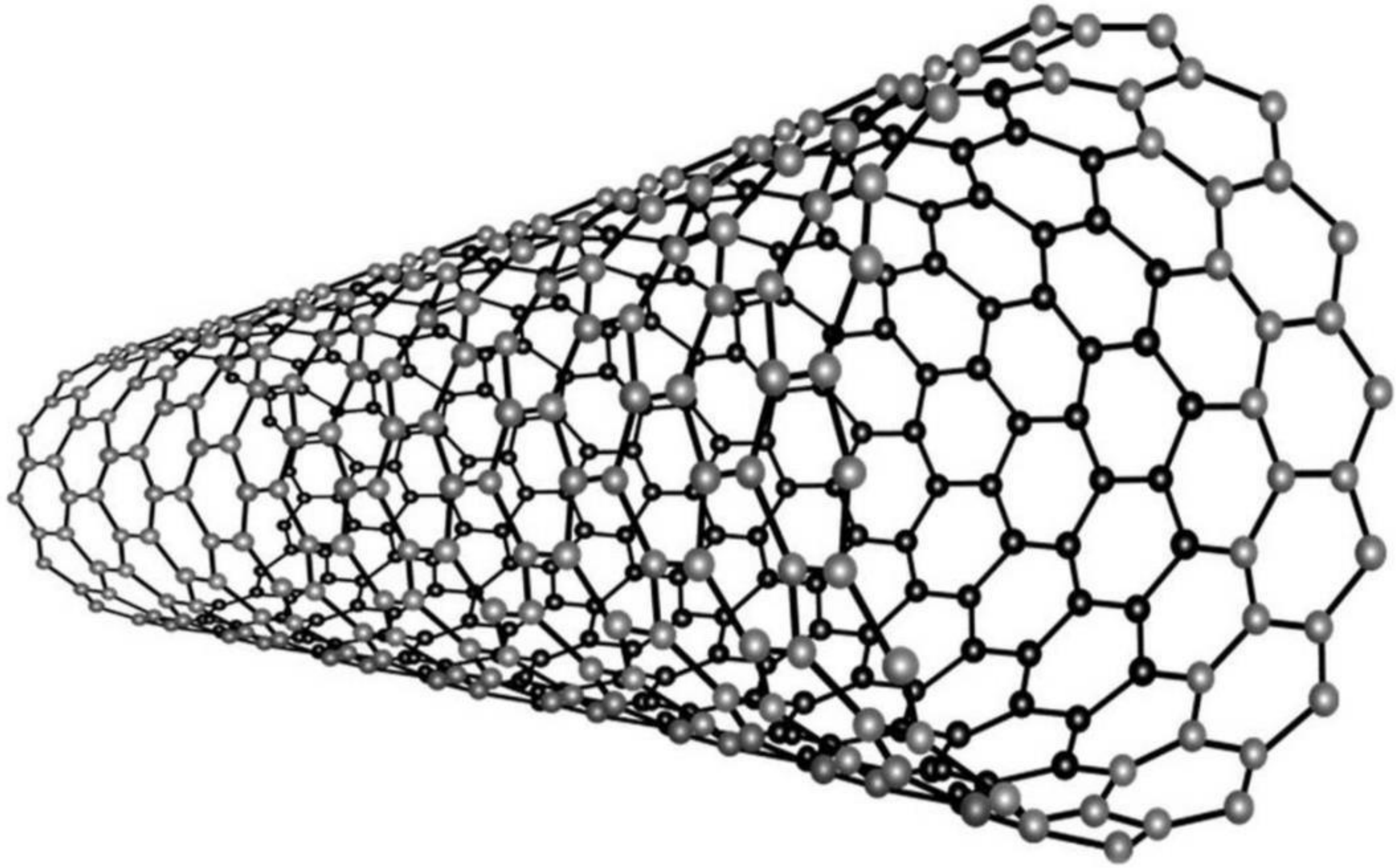
The Thomson Problem is one of 18 unsolved mathematics problems proposed by the mathematician Steve Smale.

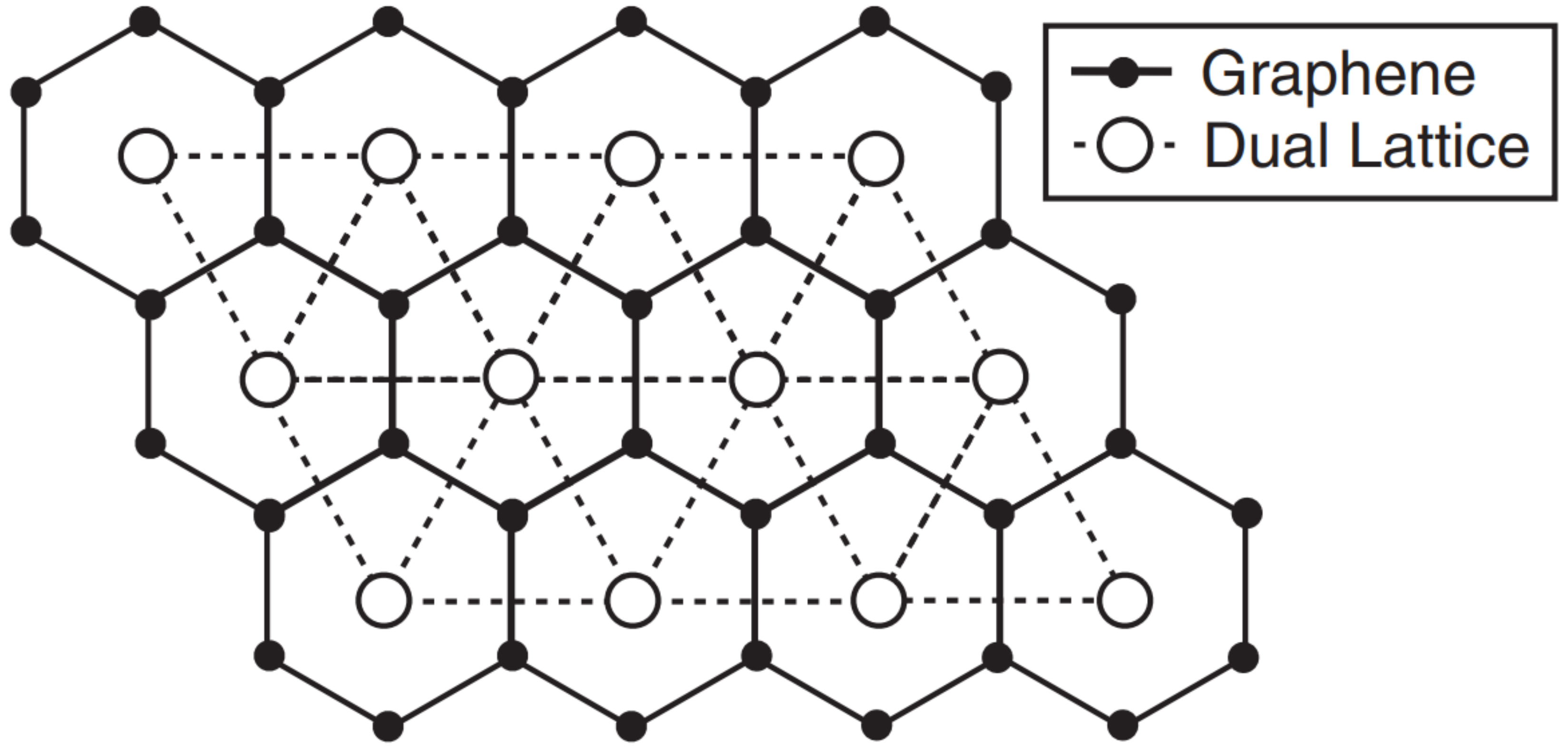
S. Smale (2000)
"Mathematical problems for the next century"

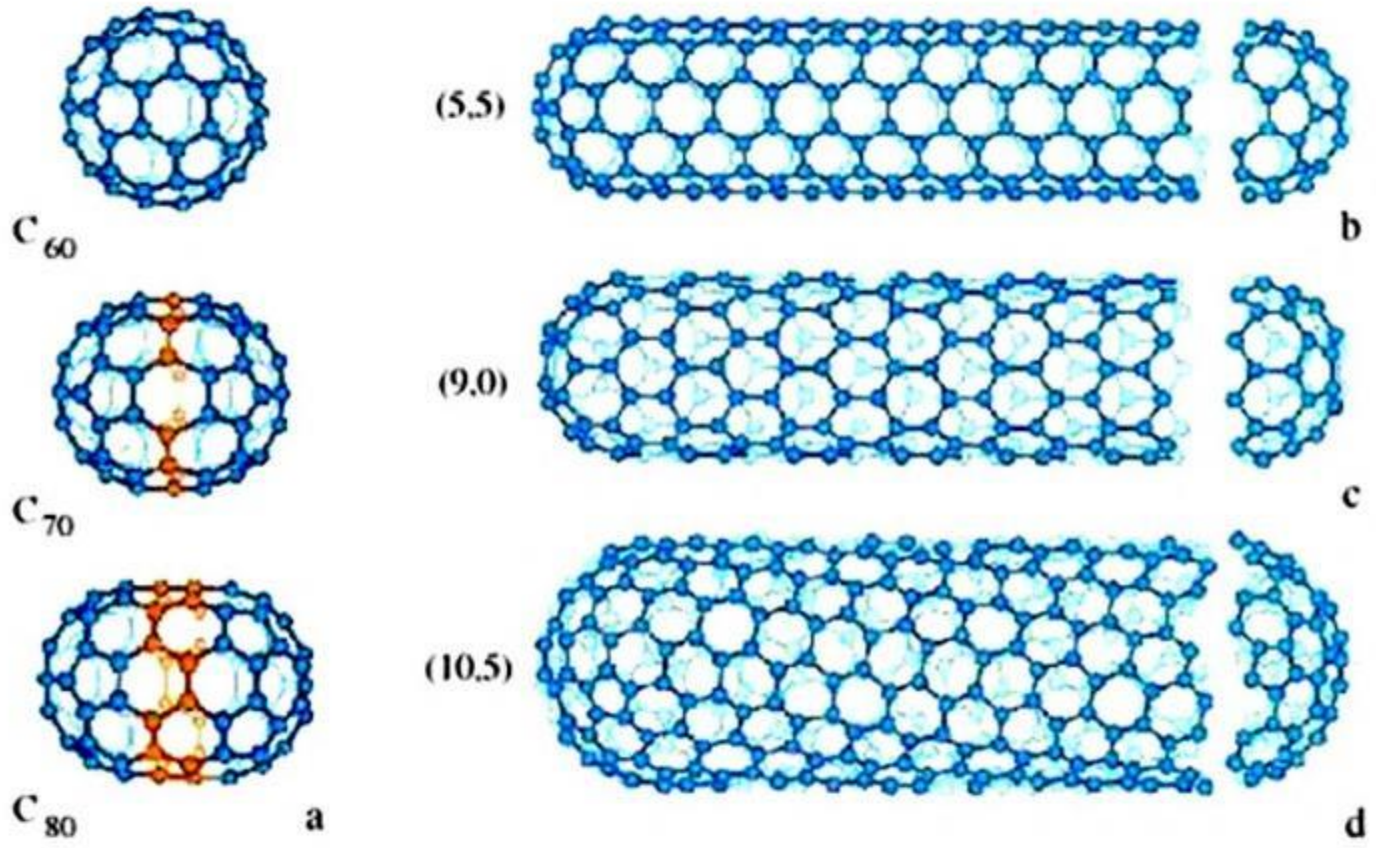
Thomson problem



The problem of coating of carbon nanotubes by suitable fullerene.







Applications of the Thomson Problem

- Strongly correlated Coulomb systems (quantum dots, dusty plasma, colloidal crystals)
- Theory of telecommunications
- The problem of determining the measure of protein subunits that form shells of spherical viruses
- New ideas on the role of geometry and topology in the theory of ordered systems
- Coding theory
- Optimization theory

Mathematical formulation of the problem

Finding values $x^{(1)}, \dots, x^{(N)} \in S$:

$$W_N = \inf_{x^{(1)},\dots,x^{(N)} \in S} W\left(x^{(1)}, \dots, x^{(N)}\right), \quad W = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{\left|r_i - r_j\right|},$$

where r_i is radius vector of point $x^{(i)} \in S$.

Analytical approaches to the Thomson problem solution

N	Extremum configuration
2	diametrically opposite points
3	equilateral triangle
4	tetrahedron
5	regular triangular bipyramid
6	regular octahedron
7, 8, 9, 10, 11	not solved
12	icosahedron
> 12	not solved

Current state of the problem

1. **"Equilibrium configurations of n equal charges on a sphere“**, T. Erber, G. M. Hockney, J Phys A: Math, **1991**.
2. **“Possible Global Minimum Lattice Configurations for Thomson's Problem of Charges on a Sphere”**.

   Altschuler, Williams, Ratner, Tipton, Stong, Dowla, Wooten. Phys. Rev. Lett. 78, 2681(**1997**)
3. **“Numerical study of the structure of metastable configurations for the Thomson problem”.**

   A. Bondarenko, T. Bugueva, L. Kozinkin. Russian Physics Journal, **2016**. DOI 10.1007/s11182-016-0746-3
4. **“Generalized method for constructing the atomic coordinates of nanotube caps”.** M. Robinson, I. Suarez-Martinez, N. Marks. Physical review 87, 155430 (**2013**)

Numerical methods for solving the Thomson problem

- **Particle Swarm Optimization**[1]
- **Broyden-Fletcher-Goldfarb-Shanno algorithm**[2]
- **Dynamic Monte Carlo simulation method**[3]

1. Kennedy, J.; Eberhart, R. (1995). **Particle Swarm Optimization**. *Proceedings of IEEE International Conference on Neural Networks*. IV. pp. 1942–1948. doi:10.1109/ICNN.1995.488968.
2. Fletcher, Roger (1987), ***Practical methods of optimization*** (2nd ed.), New York: John Wiley & Sons, ISBN 978-0-471-91547-8
3. A.N. Bondarenko, M.N. Karchevskiy and L.A. Kozinkin, **The Structure of Metastable States in The Thomson Problem**. Journal of Physics: Conference Series 643 (2015) 012103 doi:10.1088/1742-6596/643/1/012103

Graph invariants

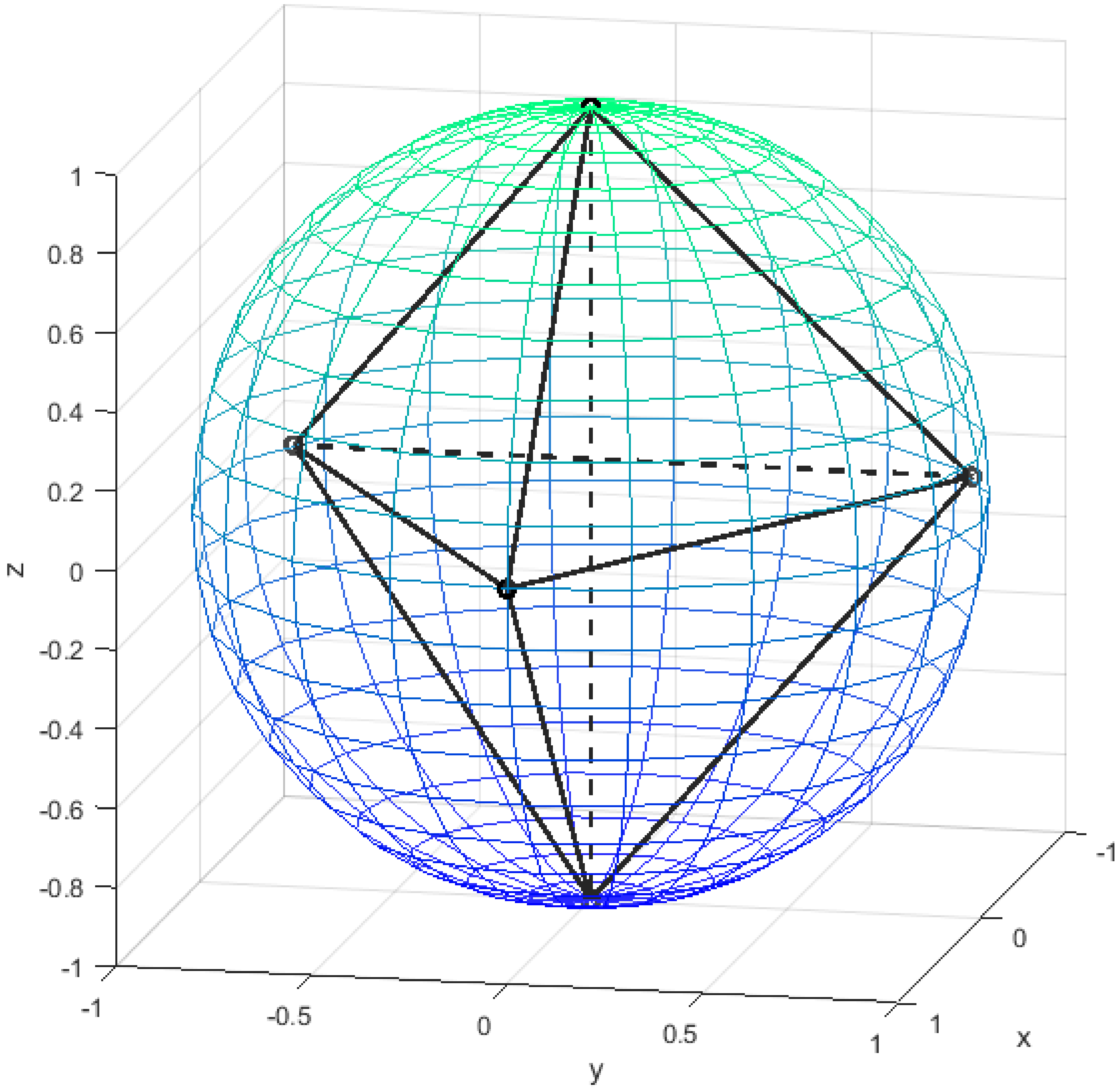
- The characteristic polynomial of the adjacency matrix
- The ordered spectrum of the graph

So far, it has not been possible to construct a complete system of polynomial-time invariants of isomorphic graphs.

A direct algorithm for verifying graph isomorphism

A **spherical graph** is a complete weighted graph whose vertices can be arranged on the unit sphere.

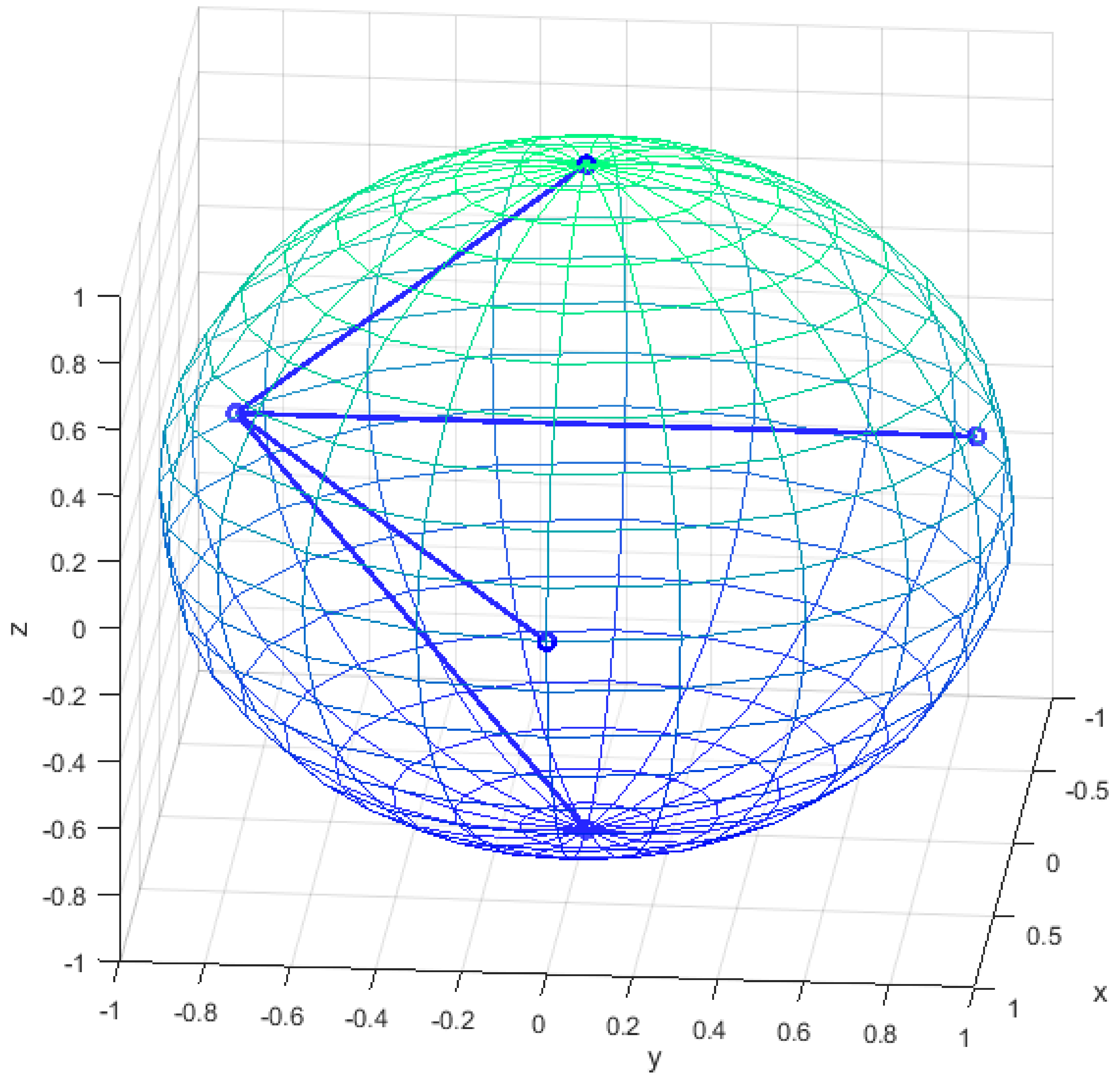
<u>Example</u>:
Thomson problem solution for N = 5



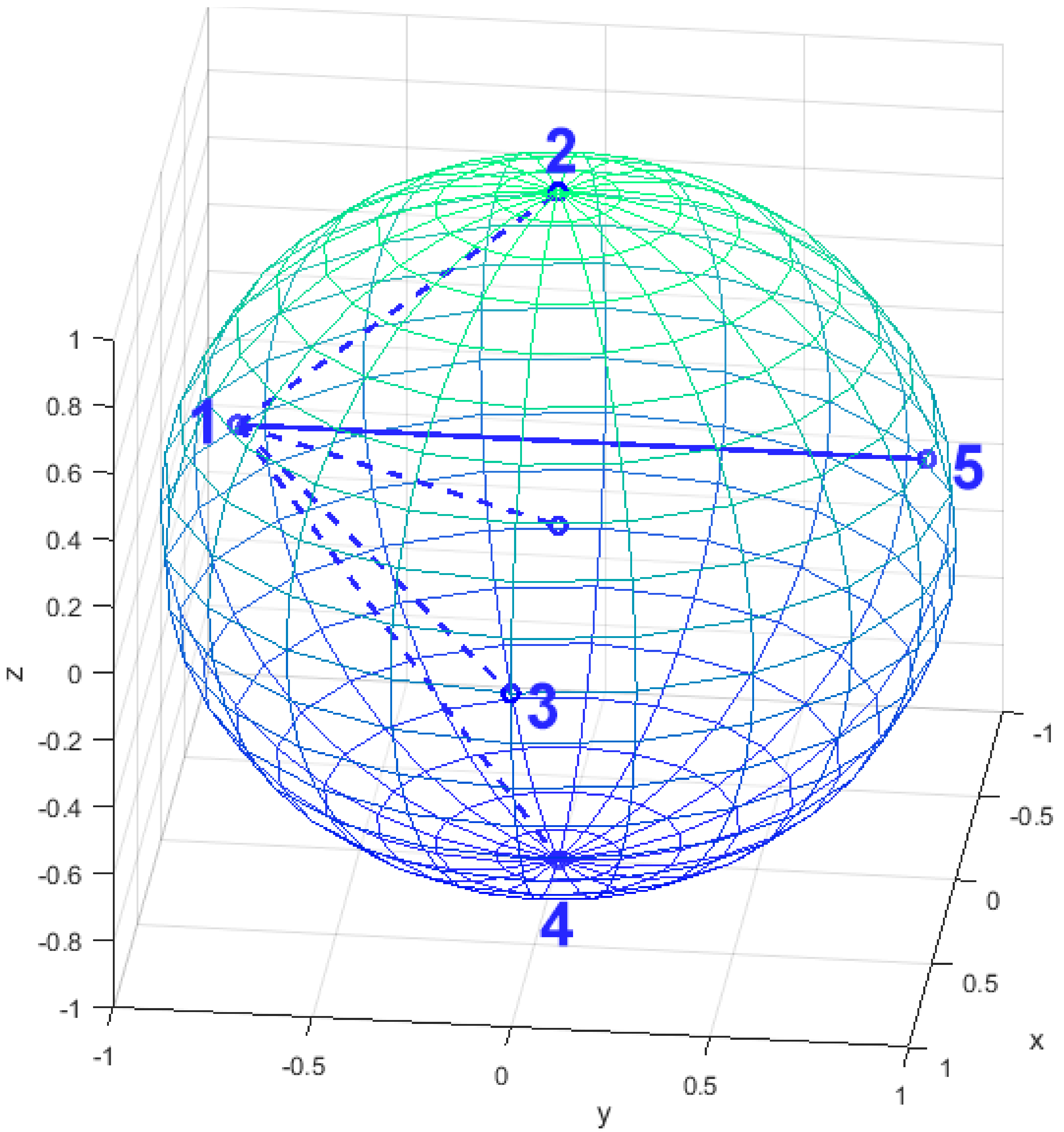
A direct algorithm for verifying graph isomorphism

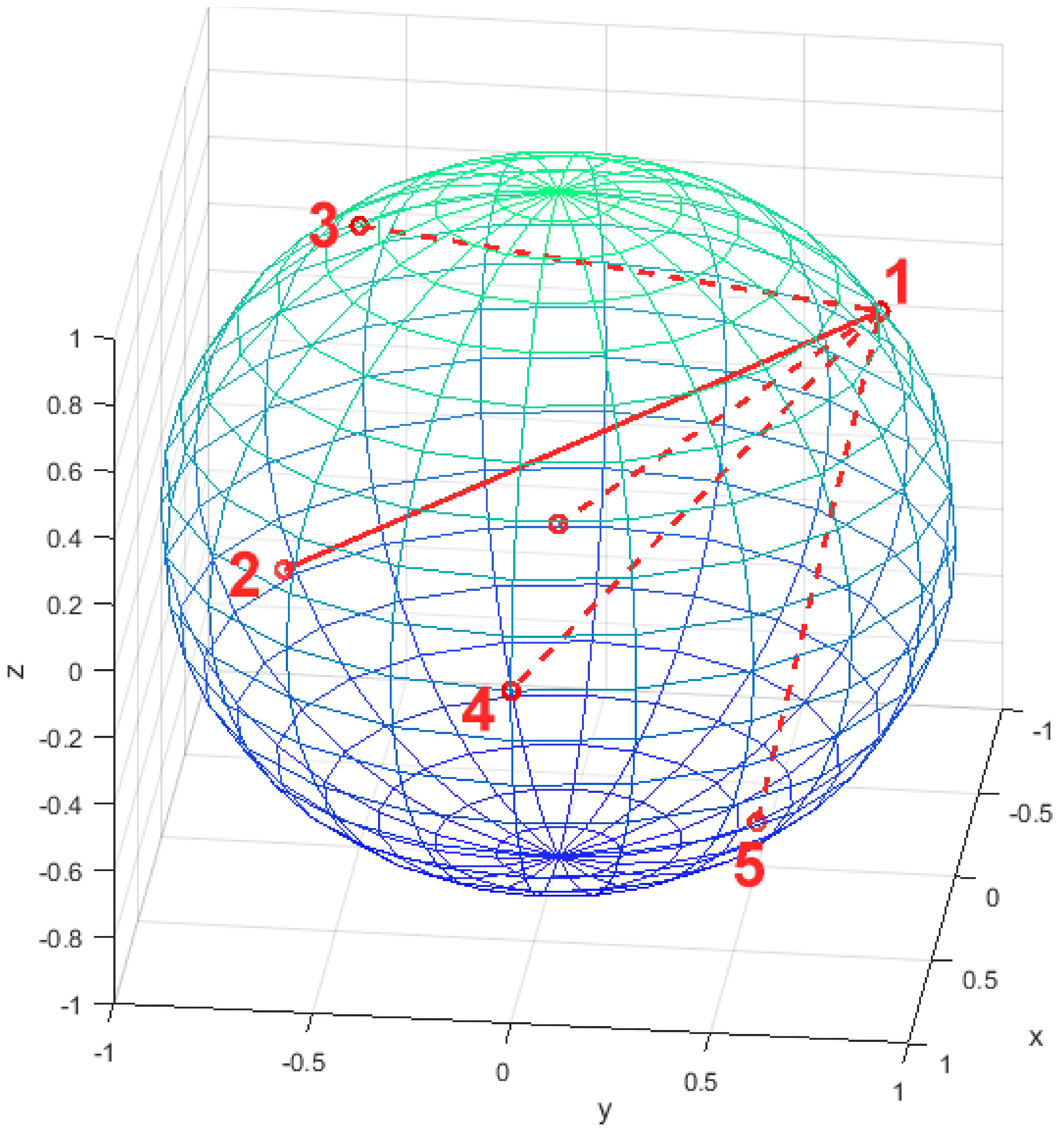
A **sheaf of spherical graph** is a set of one vertice and all edges incident to it.

<u>Example</u>:
Sheaf of spherical graph, based on the Thomson problem solution for N = 5

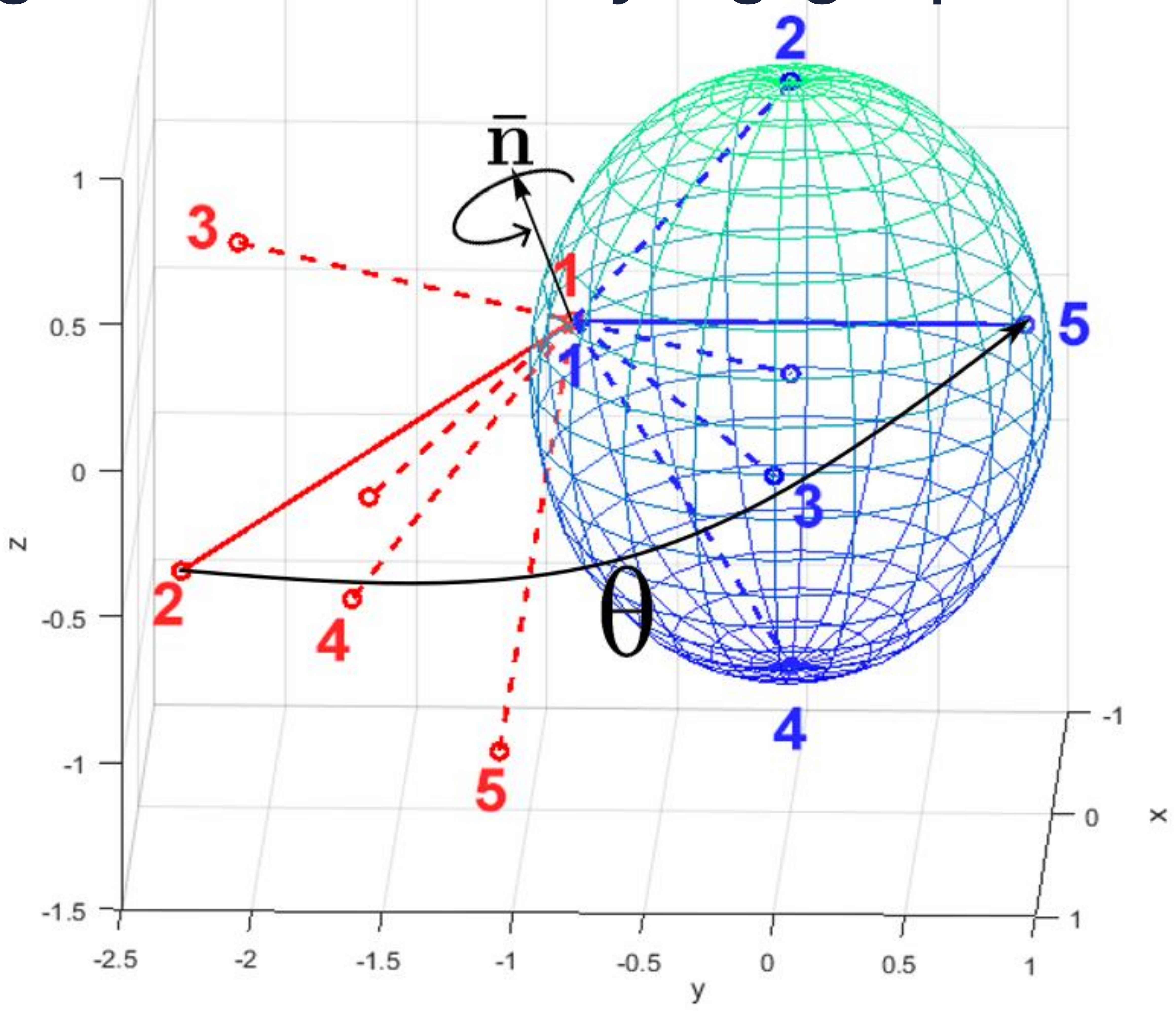


A direct algorithm for verifying graph isomorphism

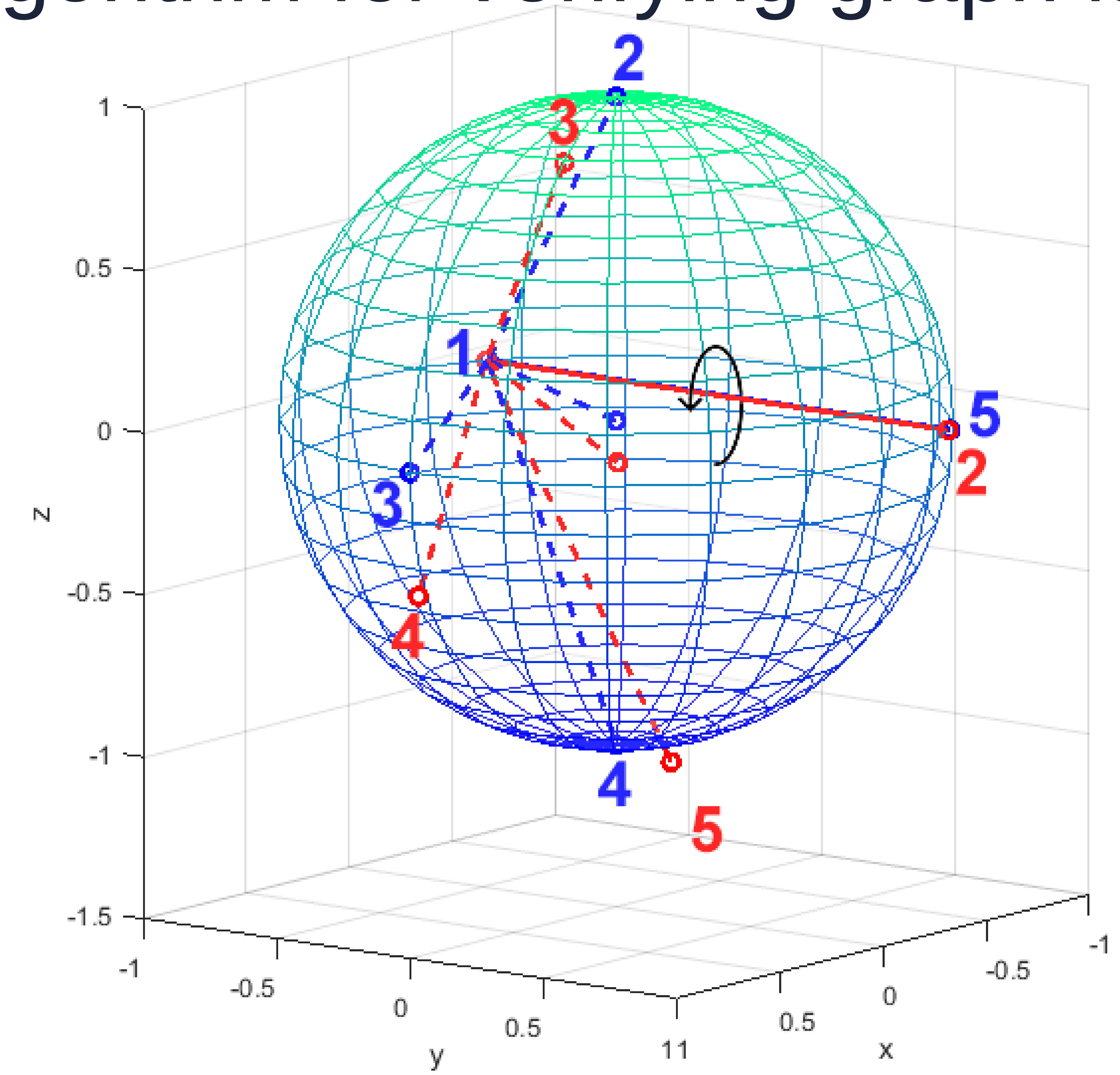




A direct algorithm for verifying graph isomorphism



A direct algorithm for verifying graph isomorphism



A direct algorithm for verifying graph isomorphism

Theorem

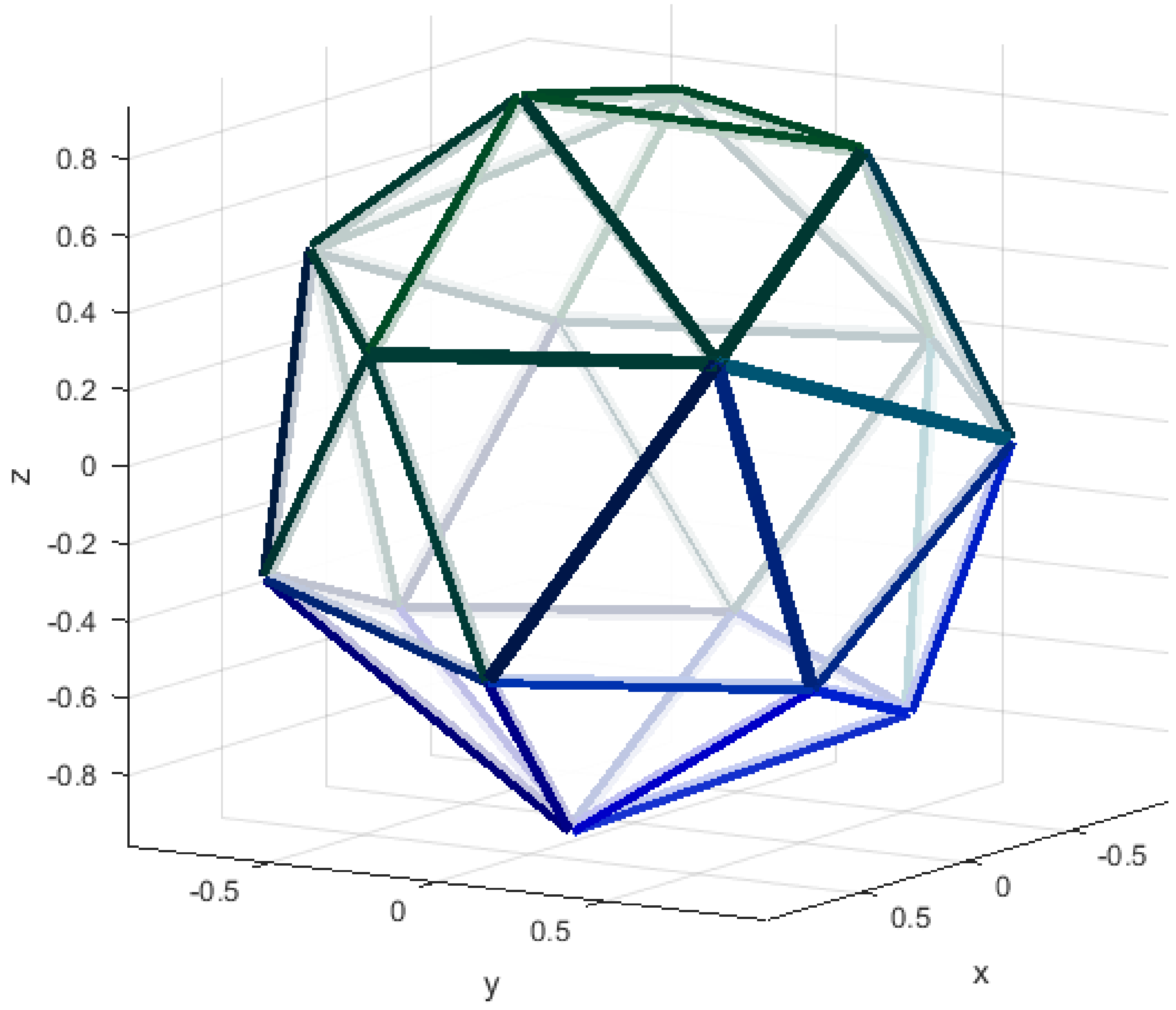
The complexity of the proposed algorithm is $O(N^5)$, where N – amount of charges.

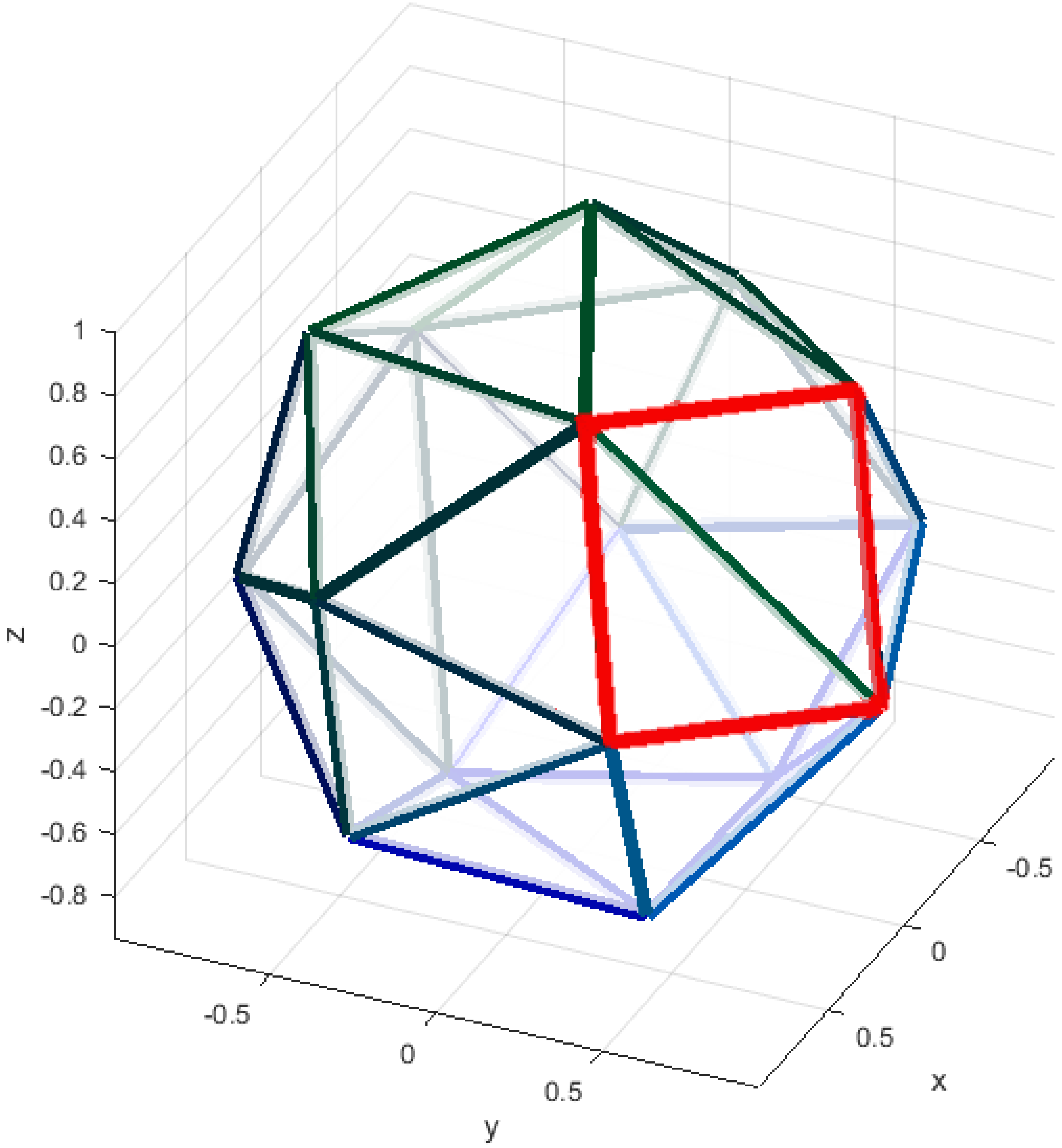
The required amount of memory: $O(N^2)$ cells.

Results of numerical simulation

N	Amount of metastable configurations	Energy
4	1	3.67424
5	1	6.48964
6	1	9.97829
7	1	14.43754
8	1	19.68272
9	1	25.75849
10	1	32.71623
11	1	40.49512
12	1	49.14637
13	1	58.86237
14	1	69.38275
15	1	80.66247
16	2	92.91062 / 92.91308

Results of numerical simulation





Conclusion

The study of the equilibrium states of the Thomson problem was carried out.

A mathematical model is presented that allows to classify solutions of the Thomson problem depending on their geometrical structure. An example of incompatible solutions is given.

The polynomial algorithm for verifying spherical graph isomorphism was constructed.

Thanks!

stepan-fadeev@mail.ru