Nucleon Clustering Modelling in Heavy Nuclei Fission Taking into Account the Coulomb Interaction

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Nuclear physics, elementary particle physics, and nuclear technologies”

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Outline

- Introduction
- Nucleon Clustering Modelling
- Simulation Results
- Nucleon Clustering Modelling Taking into Account the Coulomb Interaction
- Conclusion

Section 1

INTRODUCTION

A model with a new type of dynamics was introduced by Vicsek in order to reproduce the emergence of self-ordered motion, aggregation and clustering in systems of particles with complex interaction (Phys.Rev.Lett.75, 1995).

This compelling discrete-time model of cooperative motion shows that the nearest neighbor rule can cause some number of particles move in same direction despite the absence of centralized coordination and despite the fact that each set of nearest neighbors change with time as the system develops.

Friedkin, Noah E., Anton V. Proskurnikov, Roberto Tempo, and Sergey E. Parsegov.
Network science on belief system dynamics under logic constraints
Science 354, no. 6310 (2016): 321-326.

Vicsek-type physics is a field concerned with systems as diverse as synthetic self-propelled colloids, groups of small robots, mixtures of biofilaments and motor proteins, eukaryotic cells, swimming sperm or bacteria, and animal flocks.

A Jadbabaie, J Lin, AS Morse
Coordination of groups of mobile autonomous agents using nearest neighbor rules
IEEE Transactions on automatic control 48 (6), (2003): 988-1001

A fundamental concern for networked cooperative dynamical systems is the study of their interactions and collective behaviors under the influence of the information flow allowed in the communication network. This communication network can be modeled as a graph with directed edges or links corresponding to the allowed flow of information between the systems. The systems are modeled as the nodes in the graph and are sometimes called agents. Information in communication networks only travels directly between immediate neighbors in a graph. Nevertheless, if a graph is connected, then this locally transmitted information travels ultimately to every agent in the graph.

Various terms are used in literature for phenomena related to the collective behavior on networks of systems, such as flocking, consensus, synchronization, frequency matching, formation, rendezvous, and so on. The nature of synchronization in different groups depends on the manner in which information is allowed to flow between the individuals of the group.

The engineering study of multi-agent cooperative control systems uses principles observed in sociology, chemistry, and physics to obtain synchronized behavior of all systems by using simple local distributed control protocols that are the same for each agent and only depend on that agent’s neighbors in the group.

Graph Laplacian Potential and Multi-Agent Systems

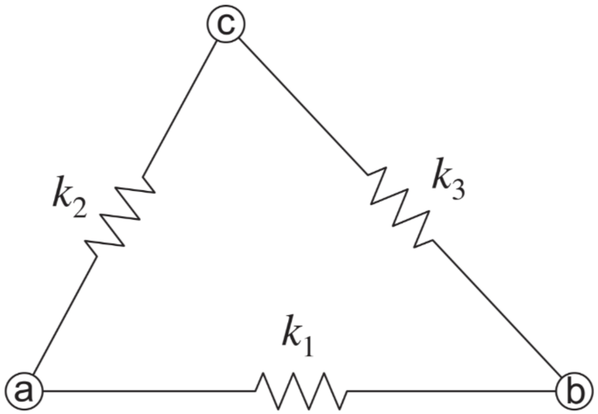
Nuclear interacting particle system could be represented by a network where the nodes stand for particles and the edges stand for interaction between the particles.

For networked multi-agent systems, there is an energy-like function, called the graph Laplacian potential, that depends on the communication graph topology. The Laplacian potential captures the notion of a virtual potential energy stored in the graph.

The system of interacting particles is described by the multi-agent system where each particle is represented by an agent. The system is modelled by a distributed network where each agent depends only on information about the agent and its neighbors.

As a kind of energy, zero Laplacian potential implies a steady-state condition of the graph, which under certain conditions is equivalent to consensus of all agents.

Networked Spring-Mass System



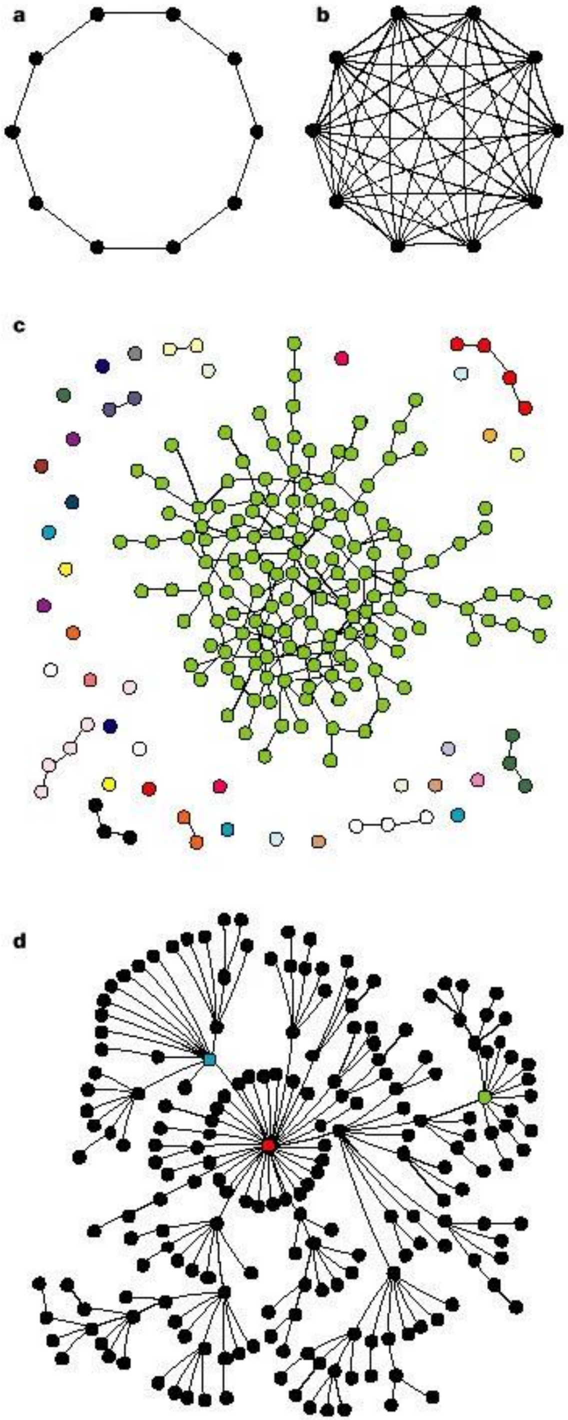
Potential energy often means the energy stored in a spring or in a potential field,
such as the gravity field or the electric field, when work is done to stretch a spring
or against the potential field.

If a spring, with the spring constant *k*, is stretched by a length of *x*, then the potential energy stored in the spring is ½ kx^2.
Consider a networked spring-mass system, three point masses linked by three springs, as shown in the Figure. Suppose the ideal free lengths of these springs are all zero. Then, the potential energy P_E stored in these springs is

$$P_E = \frac{1}{2} k_1 |\overrightarrow{ab}|^2 + \frac{1}{2} k_2 |\overrightarrow{ac}|^2 + \frac{1}{2} k_3 |\overrightarrow{bc}|^2,$$

where k_1, k_2, and k_3 are the spring constants, and *ab*, *ac*, and *bc* are the lengths between each two masses.

The “potential energy” for a multi-agent system can be treated as the virtual energy stored in a graph, and thus is called the graph Laplacian potential. In this case, the nodes are connected not by springs, but communication links with edge weights.



Strogatz SH
Exploring complex networks.
Nature 410 (2001): 268–276

“Are there any unifying principles underlying their topology? From the perspective of nonlinear dynamics, we would also like to understand how an enormous network of interacting dynamical systems — be they neurons, power stations or lasers — will behave collectively, given their individual dynamics and coupling architecture”

Section 2

NUCLEON CLUSTERING MODELLING

Extended Vicsek-type Model

$$x_i^{t+1} = x_i^t + z_i^t + \gamma_a \sum_{j \in N_i^t} ca_{ij}^t (x_j^t - x_i^t) - \gamma_r \sum_{j \in N_i^t} cr_{ij}^t (x_j^t - x_i^t)$$

The state x_{i+1}^t of the ith particle at time instant $t+1$ is equal to its state x_i^t at the previous moment at time instant t, plus the influence of external disturbance z_i^t, plus the influence of interaction with neighboring particles $j \in N_i^t$, where N_i^t is the set of neighboring particles of particle i at time t.

$$ca_{ij}^t = \begin{cases} 1, & \text{if there is an attraction between particles } i \text{ and } j \\ 0, & \text{otherwise} \end{cases}$$

$$cr_{ij}^t = \begin{cases} 1, & \text{if there is a repulsion between particles } i \text{ and } j \\ 0, & \text{otherwise} \end{cases}$$

γ_a and γ_r are attraction and repulsion coefficients correspondingly.

Multiagent System

Multiagent systems recently have become a popular tool in modelling and studying of complex natural and societal processes.

In a complex system composed of a large amount of elements (agents) a clustering phenomenon is an interesting subject for investigation.

For instance, it could allow to describe a state or behaviour of complex system in a simpler way.

Agent Dynamics

Assume agent i is described by its state x_i^t. Consider a set of agents N, that are connected in some way. The connections could be given in terms of graphs. Construct graph $G = \{N, E^t, C^t\}$ where the set of nodes N stands for the particles, set of edges E^t denotes inter-agent connections, and matrix C^t is an adjacency (or connectivity) matrix of graph G.

i-th agent state dynamics can be described by equation:

$$x_i^{t+1} = x_i^t + z_i^t + u_i^t, \quad (1)$$

where z_i^t stands for the disturbance (external or internal) affecting the agent; and u_i^t stands for the change of the agents state due to interaction with the connected agents.

Agent Interaction

Clustering in a system occurs when some groups of agents synchronize their characteristics.
An interaction between agents leading to synchronization of their states could be as follows:

$$u_i^t = \gamma \sum_{j=1}^{N} c_{i,j}^t (x_j^t - x_i^t),$$

where $\gamma \in [0,1]$ is the gain coefficient, and $c_{i,j}^t$ is the element of a connectivity matrix C^t:

$$c_{i,j}^t = \begin{cases} 1, & \text{there is a connection between agents } i \text{ and } j \\ 0, & \text{otherwise} \end{cases}$$

In simple words, agent i "looks" at its neighbors and adjusts its own state according to the average of the neighbors' states.

Graph Laplacian

Denote $L(C) = \mathrm{diag}(C \cdot \mathbf{1}) - C$ graph Laplacian,
where C is an adjacency matrix of graph G, $\mathbf{1}$ is a vector with all elements equal 1, $C \cdot \mathbf{1}$ is a vector consisting of row-sums of matrix C, $\mathrm{diag}(C \cdot \mathbf{1})$ is a diagonal matrix with elements of vector C on the diagonal.

Graph Laplacian plays an important role in analysis of multiagent system since its properties describe the system behaviour.

λ_2 is the second largest eigenvalue (also called Fiedler eigenvalue) which characterizes the connectivity of graph G. The larger number of edges in graph G are present, the larger value λ_2 takes.

Another important property of graph Laplacian is the number of its zero eigenvalues. This number corresponds to the number of the graph components (or connected subgraphs of graph G).

Multiagent System Dynamics

A system of agents' states dynamics $x_i^{t+1} = x_i^t + z_i^t + u_i^t$ can be written in vector-matrix form:
$x_i^{t+1} = x_i^t + z_i^t + u_i^t$
$x_i^{t+1} = x_i^t + z_i^t + \gamma \sum_{j=1}^N c_{i,j}^t (x_j^t - x_i^t)$
$x_i^{t+1} = x_i^t + z_i^t + \gamma \sum_{j=1}^N c_{i,j}^t x_j^t - \gamma \sum_{j=1}^N c_{i,j}^t x_i^t$
Denote $X^t = (x_1^t, \dots x_n^t)^T$, $Z^t = (z_1^t, \dots z_n^t)^T$ vectors, consisting of stacked up (vector or scalar) agents' states x_i^t and disturbances z_i^t.
$X^{t+1} = X^t + Z^t + \gamma C^t X^t - \mathrm{diag}(\gamma C^t \cdot \mathbf{1}))X^t$
using the notion of graph Laplacian we get:
$X^{t+1} = X^t + Z^t - \gamma L(C^t) X^t$

$$X^{t+1} = (I - \gamma L(C^t))X^t + Z^t. \qquad (2)$$

Assumptions

Consider the following assumptions for a basic result in multiagent system behaviour.

A1 Graph G has a spanning tree (i.e. it is connected).

A2 disturbances z_i^t and inter-agent connection occurrence $c_{i,j}^t$ are random variables independent of each other; $z_i^t, \; i = 1 \dots N$ are i.i.d; $c_{i,j}^t, \; i = 1 \dots N$ are i.i.d; z_i^t are zero mean with bounded variance σ_z, variance of $c_{i,j}^t$ is bounded.

A3 gain coefficient $\gamma < \frac{1}{\lambda_2(Q)}$,
where matrix $Q = \mathbb{E}\left(\left(L(C^t) - \mathbb{E}L(C^t)\right)^T \left(L(C^t) - \mathbb{E}L(C^t)\right) \right)$ can be thought of as "variance" of $L(C^t)$.

Theorem

If Assumptions **A1–A3** are satisfied **then** for trajectory of system (2) the following inequality holds:

$$\mathbb{E}||X^{t+1} - \bar{X}^{t+1}\mathbf{1}_n||^2 \leq \frac{\Delta}{\rho} + (1-\rho)^t \left(||X^0 - \bar{X}^0\mathbf{1}_n||^2 - \frac{\Delta}{\rho} \right),$$

where $\mathbf{1}_n$ is n-vector of ones,

$$\rho = \gamma Re(\lambda_2(L(C^t))) - \gamma^2 \lambda_{\max}(Q),$$

$$\Delta = n\sigma_z^2,$$

and $\bar{X}^t$ is a trajectory of the averaged system $\bar{X}^t = \mathbf{1}_n \cdot \frac{1}{n}\sum_{i=1}^n x_i^t$.

In short, the theorem states that in case gain γ is not too large (agents do not “overreact”), all assumptions regarding random variables are satisfied, and the network graph is connected, all agents synchronize their states.

If assumption **A1** is not met (i.e. the graph is not connected), but other assumptions are satisfied, the clustering behaviour takes place. We can consider different graph components as separate systems that will reach synchronization.

Considered Model

Assume vector $x_i \in \mathbb{R}^m$ denotes the characteristics of particle $i \in \mathcal{N}$. Neighboring particles in a considered volume interact with each other. The connections among the neighboring particles could be represented by graph $\mathcal{G} = \{\mathcal{N}, \mathcal{E}^t, C^t\}$. But the model should also account for particle repulsion that occurs at close distance. We consider two connectivity matrices: Ca^t denoting "attraction neighbors" (i.e. neighboring particles that are attracted but are not too close to be repelled) and Cr^t denoting repulsion connections of the particles that are close enough to be affected by repulsion forces.

Model Parameters

The considered model have the following parameters.

- Set of vertices $\mathcal{N}$ denoting particles i, $i \in N$.
- Attraction connectivity matrix Ca^t with elements $ca^t_{i,j} = 1$ in case the particles i and j are attracted but not too close to be repelled and $ca_{ij} = 0$ otherwise. Ca^t is constructed based on radius of attraction r_a and radius of repulsion r_r.
- Repulsion connectivity matrix Cr^t with elements $cr^t_{i,j} = 1$ in case the particles i and j are close enough to be repelled and $cr_{ij} = 0$ otherwise. Cr^t is constructed based on radius of repulsion r_r.
- Attraction and repulsion gain coefficients γ_a and γ_r that account for the relative values of attraction and repulsion forces.
- An external disturbance z_i affecting particle x_i.

System Dynamics Model

The dynamics of the system of particles is given by the following set of $\mathcal{N}$ equations in discrete time:

$$x_i^{t+1} = x_i^t + z_i^t + \gamma_a \sum_{j \in N_i^t} ca_{ij}^t (x_j^t - x_i^t) - \gamma_r \sum_{j \in N_i^t} cr_{ij}^t (x_j^t - x_i^t).$$

Define the $\mathbb{R}^{nm}$-valued vectors $\mathbf{X}_t = \{x_1, \ldots, x_m\}$ and $\mathbf{Z}_t = \{z_1, \ldots, z_m\}$ composed of corresponding vectors x_t^i and z_t^i. The system dynamics in matrix form:

$$X_{t+1} = X_t + (I - \gamma L(Ca^t) + \gamma L(Cr^t))X^t + Z^t.$$

Section 3

SIMULATION RESULTS

Nucleon Clustering Modelling ^{132}Sn

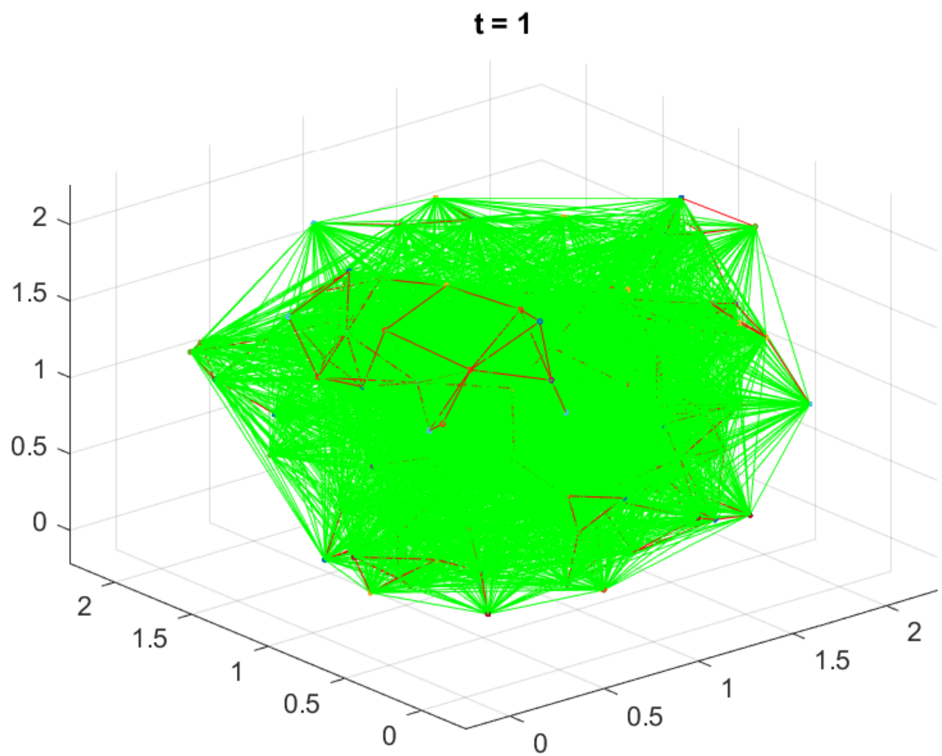
A = 132; — number of particles
Z = 50; — number of protons
T = 80; — simulation time (number of time instants)

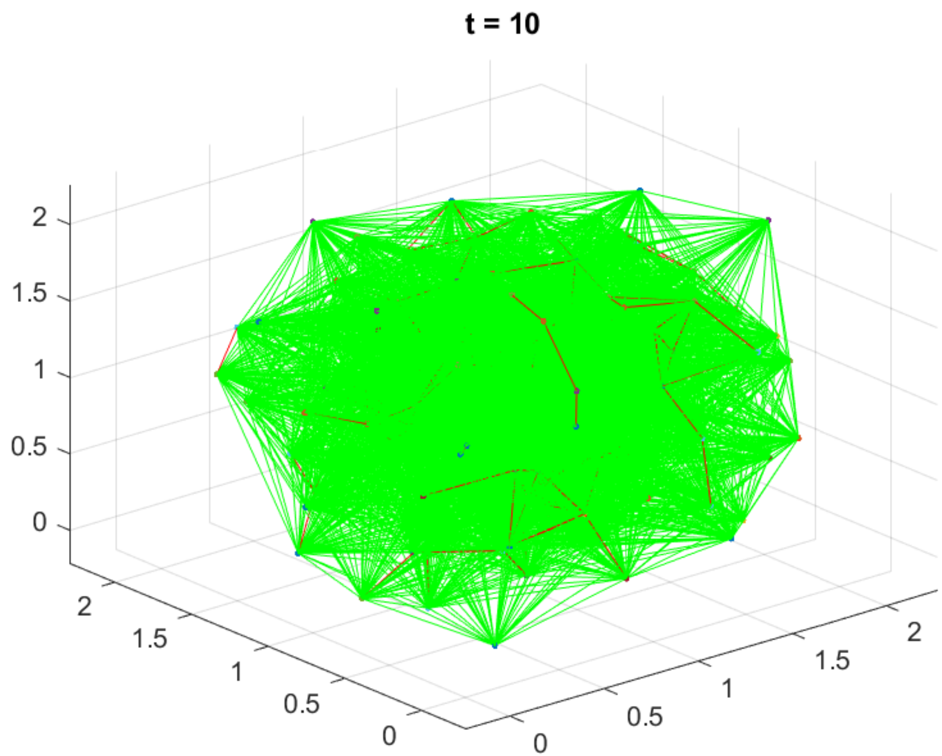
r_attr = 2; — radius of particle attraction
r_rep = 1; — radius of particle repulsion

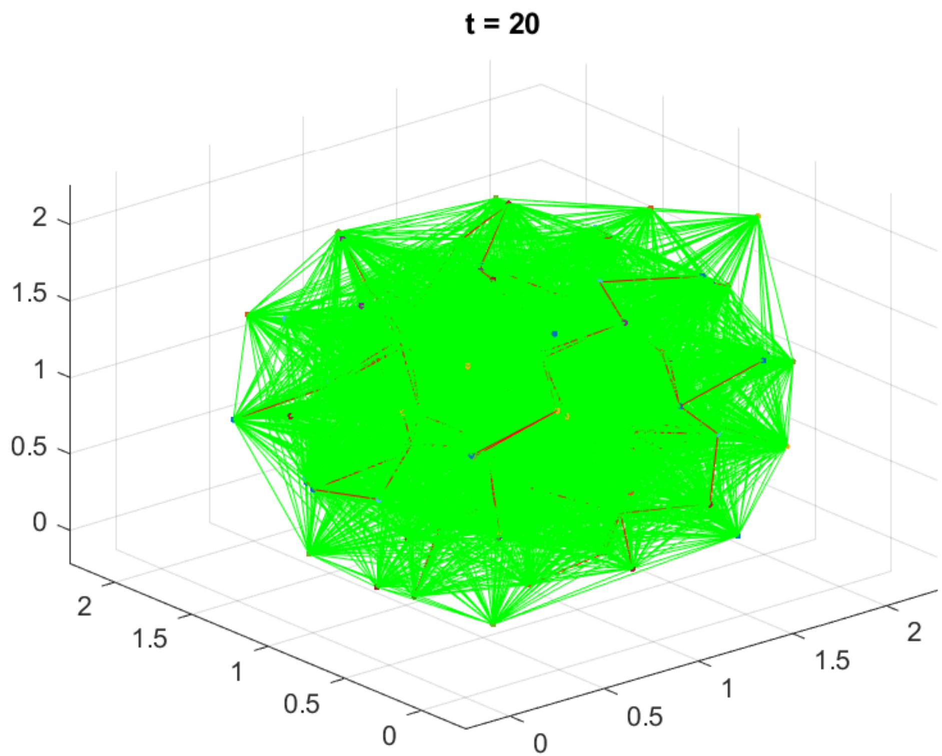
gamma_attr = 0.001; — scale parameter of particle attraction
gamma_rep = 0.1; — scale parameter of particle repulsion

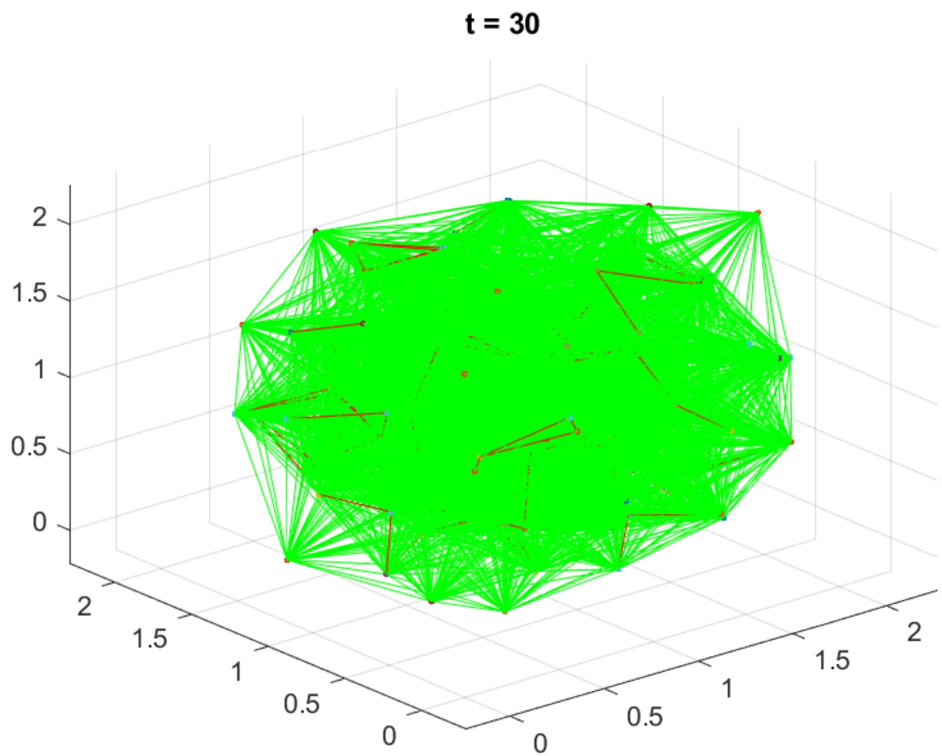
initial values of particle parameter values are set randomly
Z — particle parameter values fluctuation
simulation: small constant disturbance,

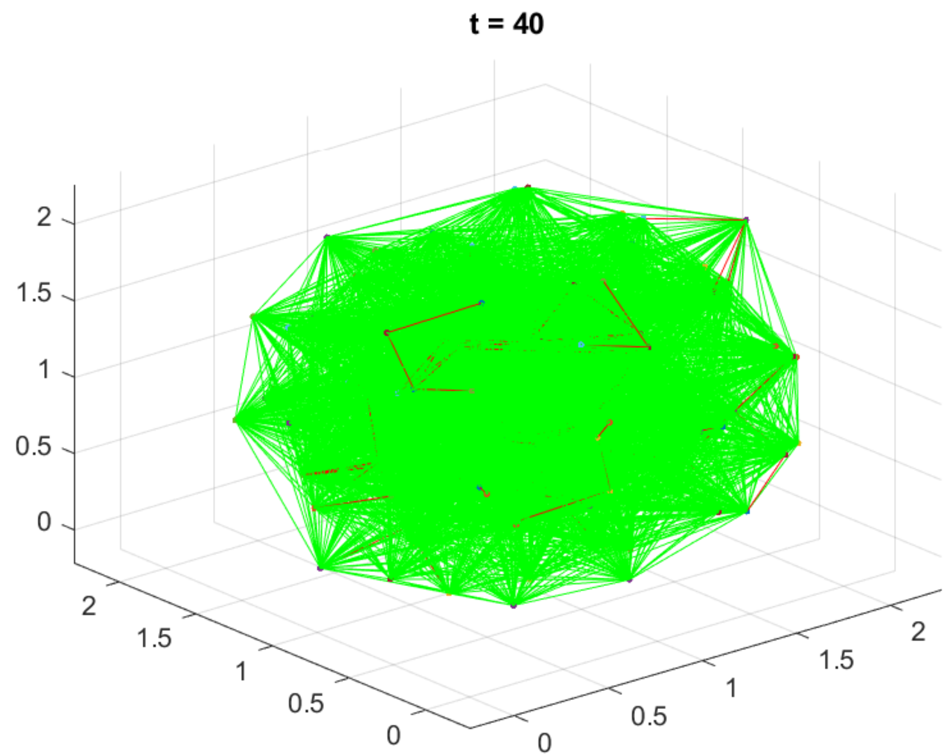
$Z \in [-0.001, 0.001]$;


t = 1
2
1.5
1
0.5
0
2
1.5
1
0.5
0
0
0.5
1
1.5
2

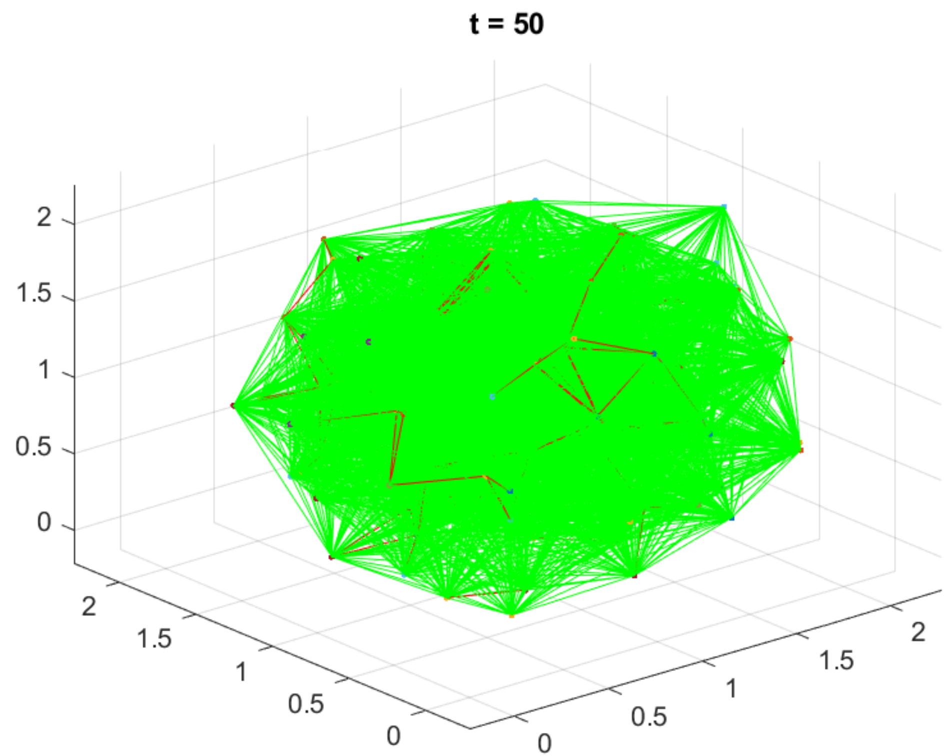

t = 10
2
1.5
1
0.5
0
2
1.5
1
0.5
0
0
0.5
1
1.5
2


t = 20
2
1.5
1
0.5
0
2
1.5
1
0.5
0
0
0.5
1
1.5
2

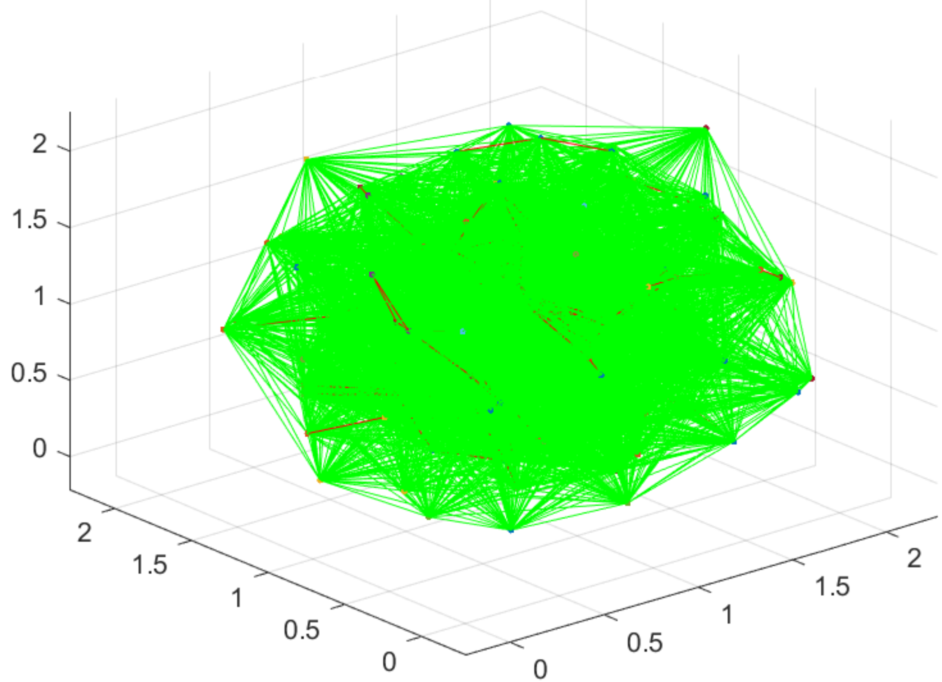

t = 30
2
1.5
1
0.5
0
2
1.5
1
0.5
0
0
0.5
1
1.5
2

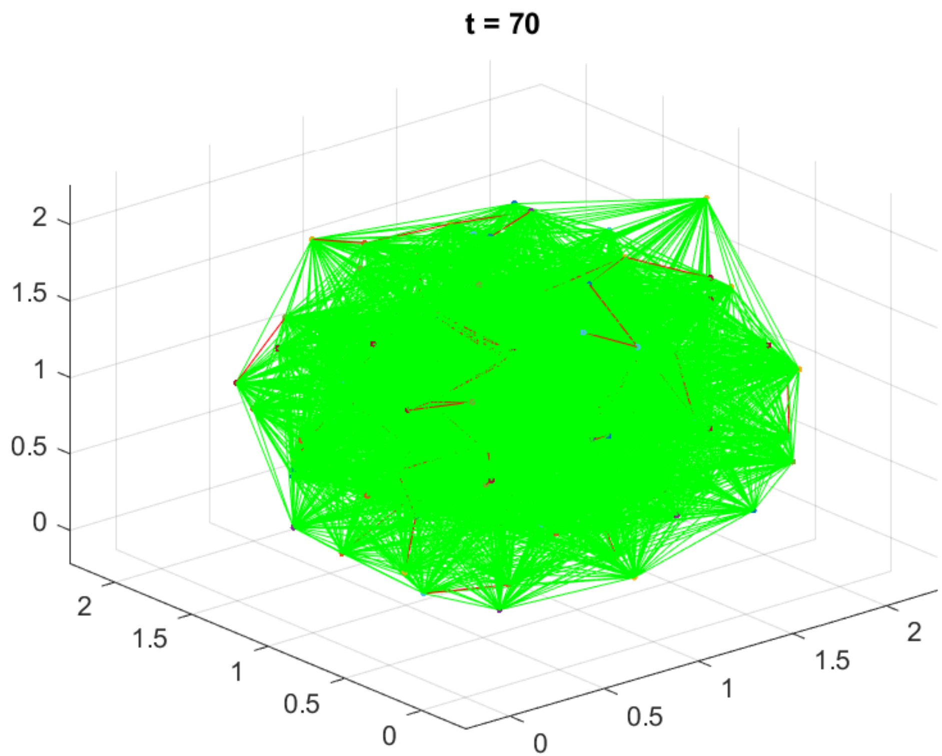


t = 40
2
1.5
1
0.5
0


t = 50
2
1.5
1
0.5
0
2
1.5
1
0.5
0
0
0.5
1
1.5
2

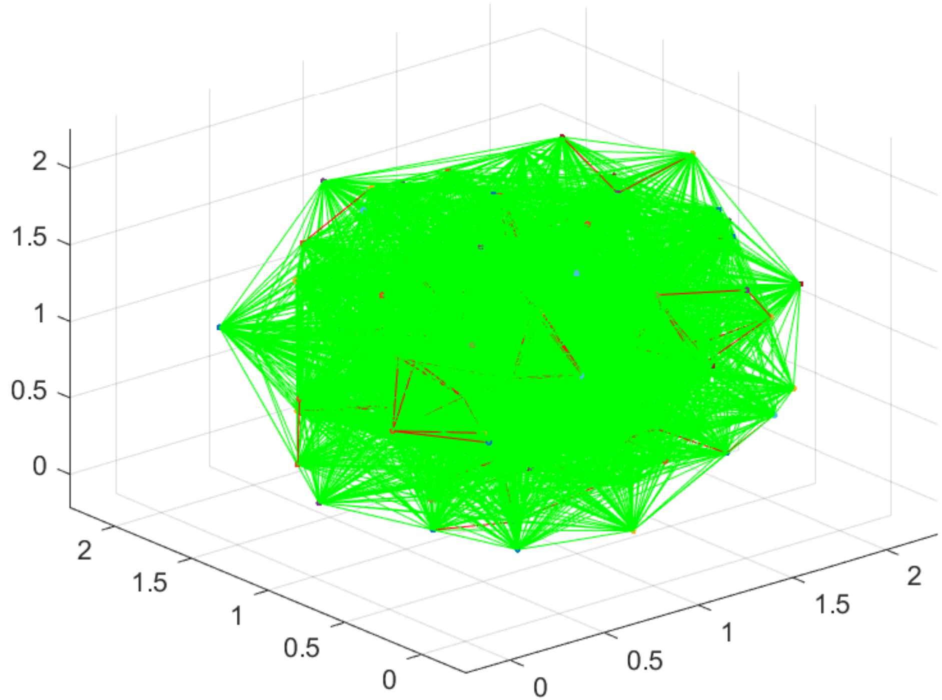
t = 60



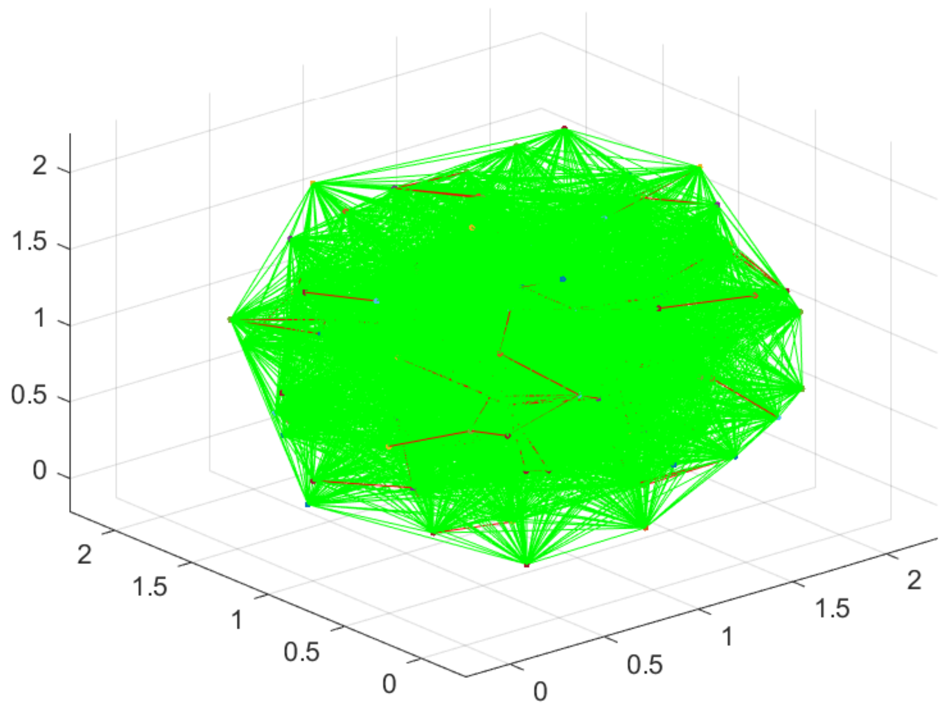


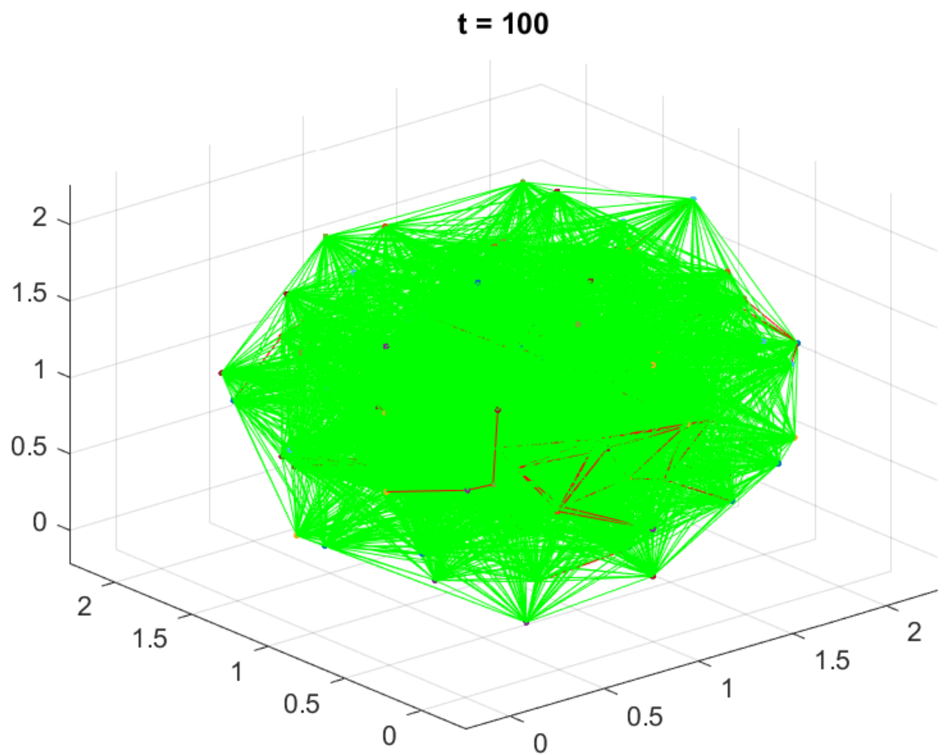
t = 70
2
1.5
1
0.5
0
2
1.5
1
0.5
0
0
0.5
1
1.5
2

t = 80

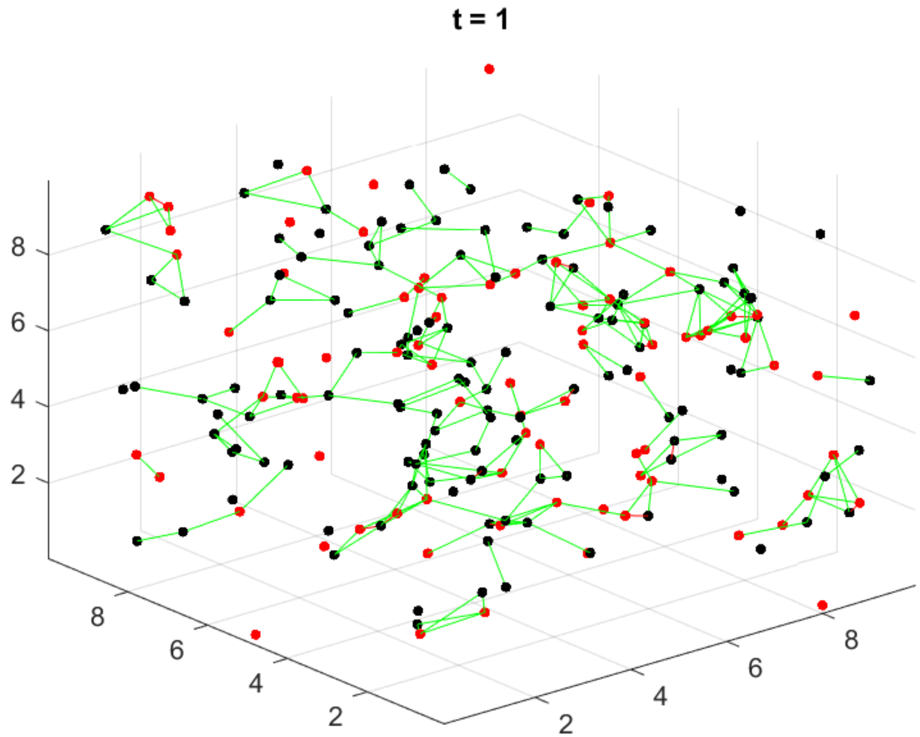


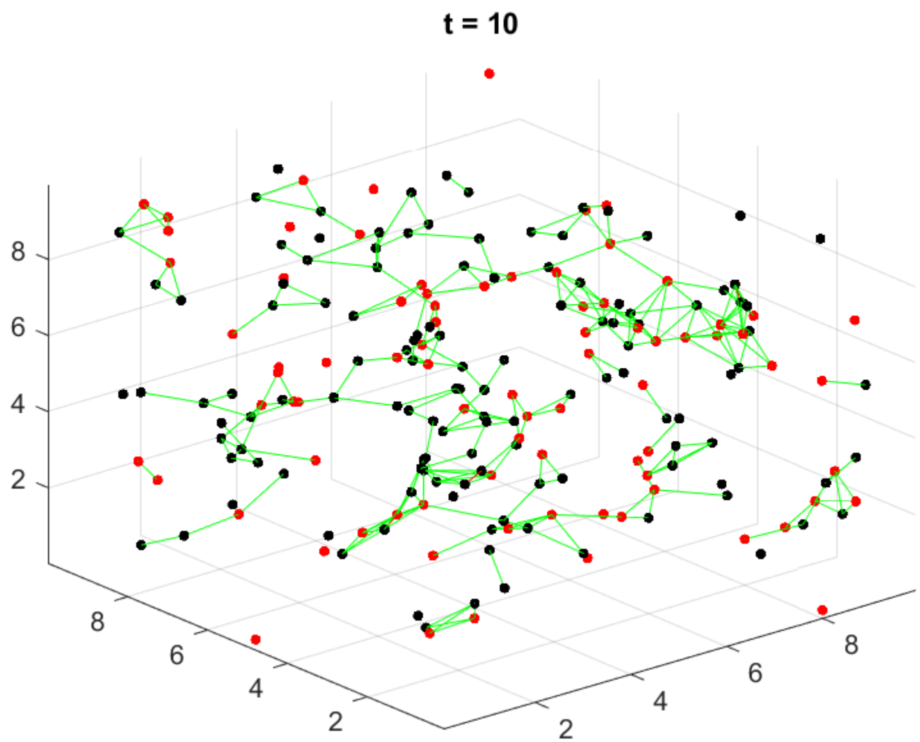
t = 90




t = 100
2
1.5
1
0.5
0
2
1.5
1
0.5
0
0
0.5
1
1.5
2

Nucleon Clustering Modelling ^{208}Pb

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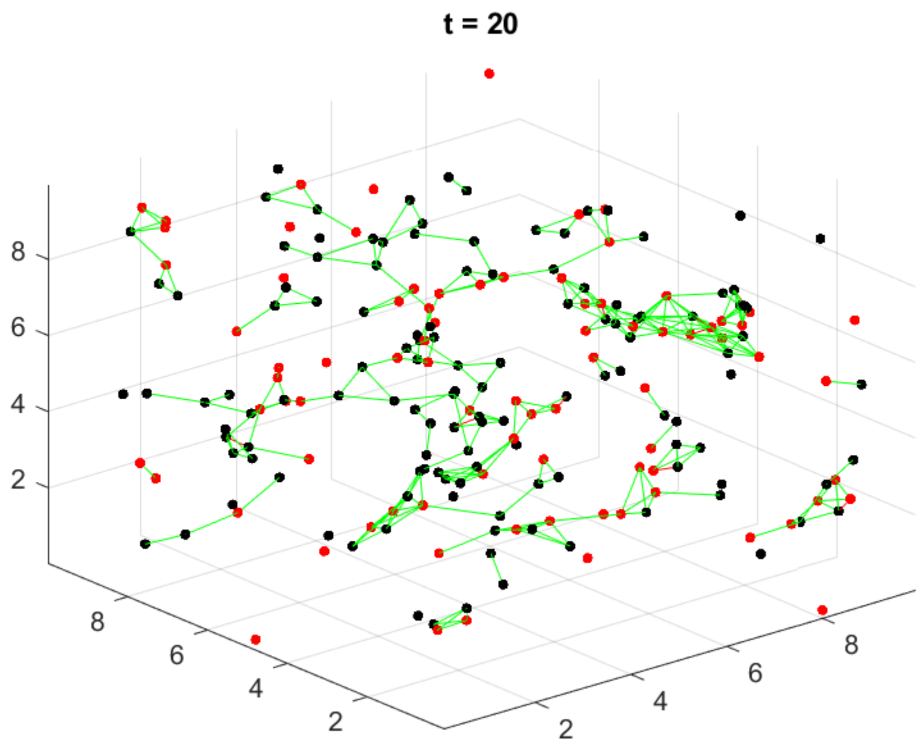
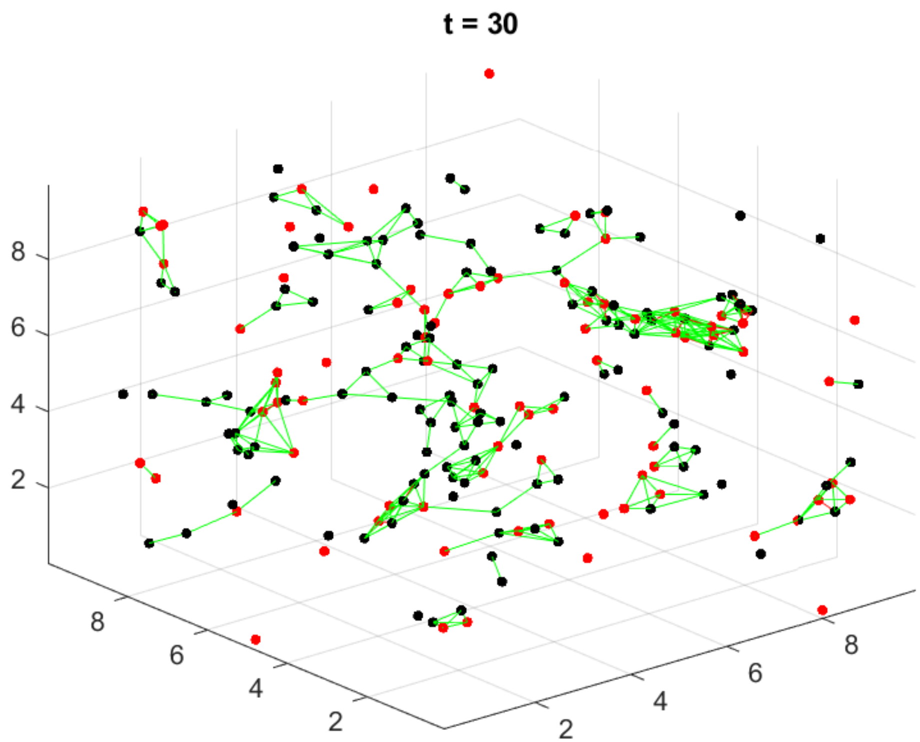
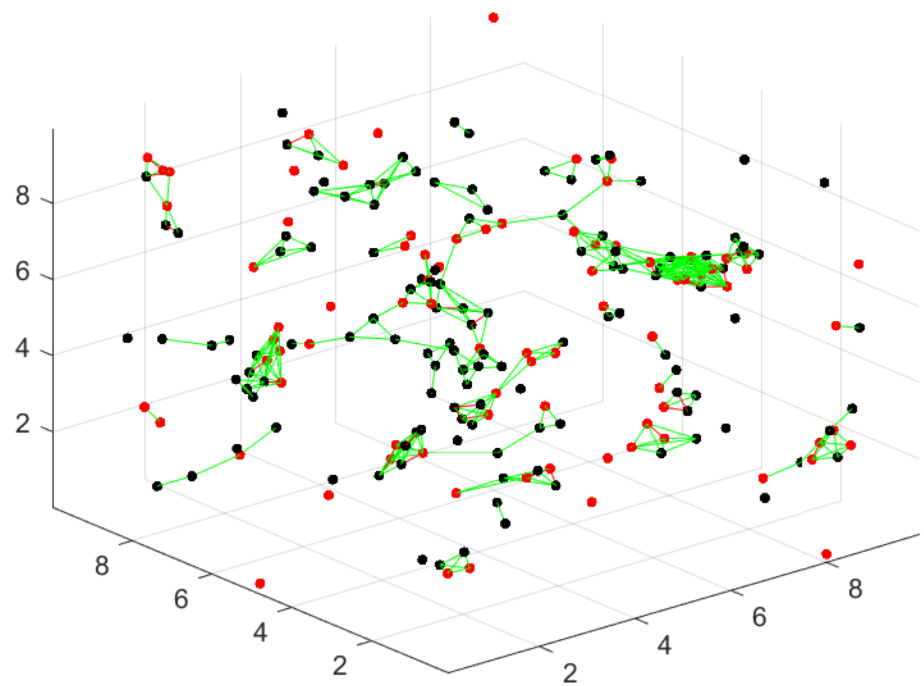
8
6
4
2
8
6
4
2
2
4
6
8

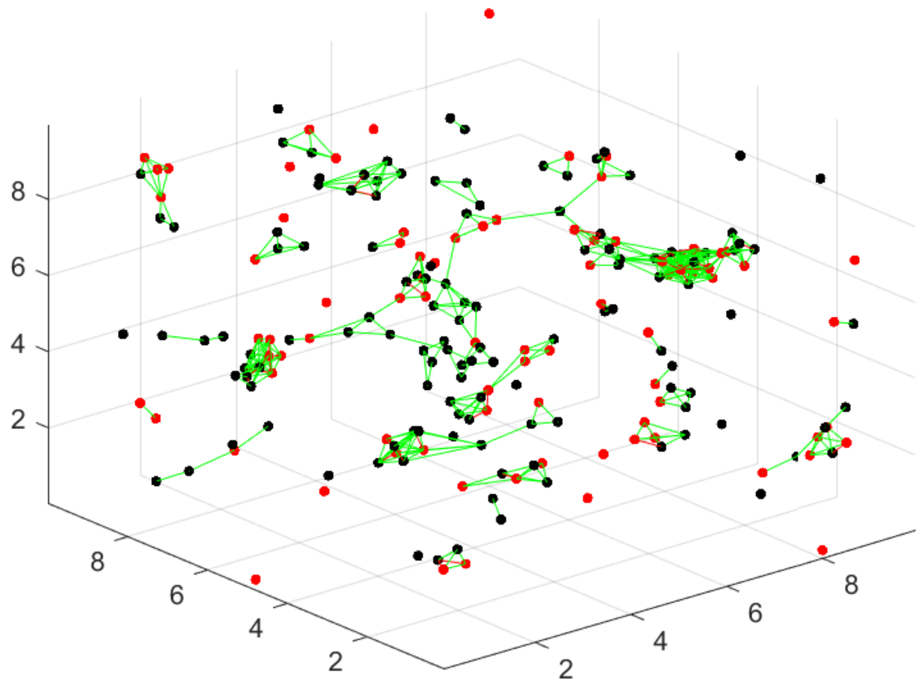

t = 20
8
6
4
2
8
6
4
2
2
4
6
8

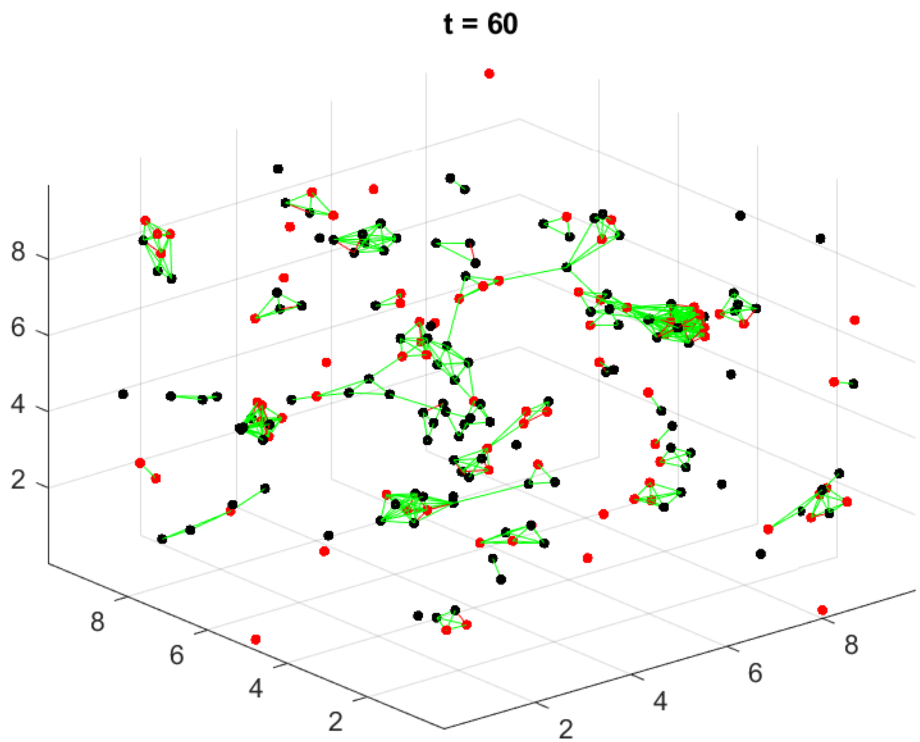

t = 30
8
6
4
2
8
6
4
2
2
4
6
8

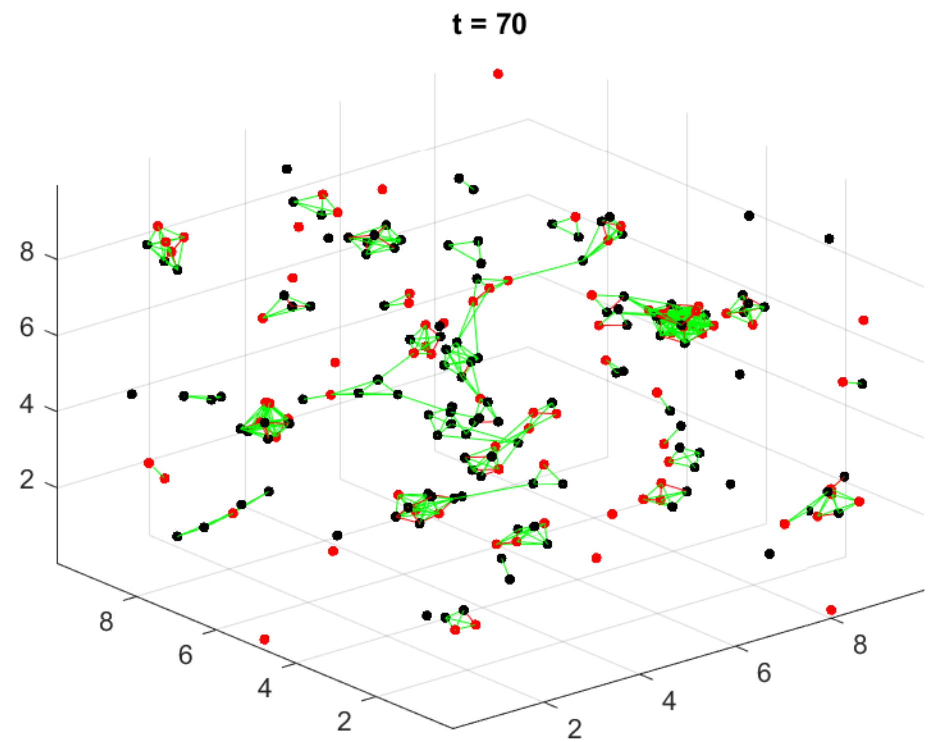
t = 40



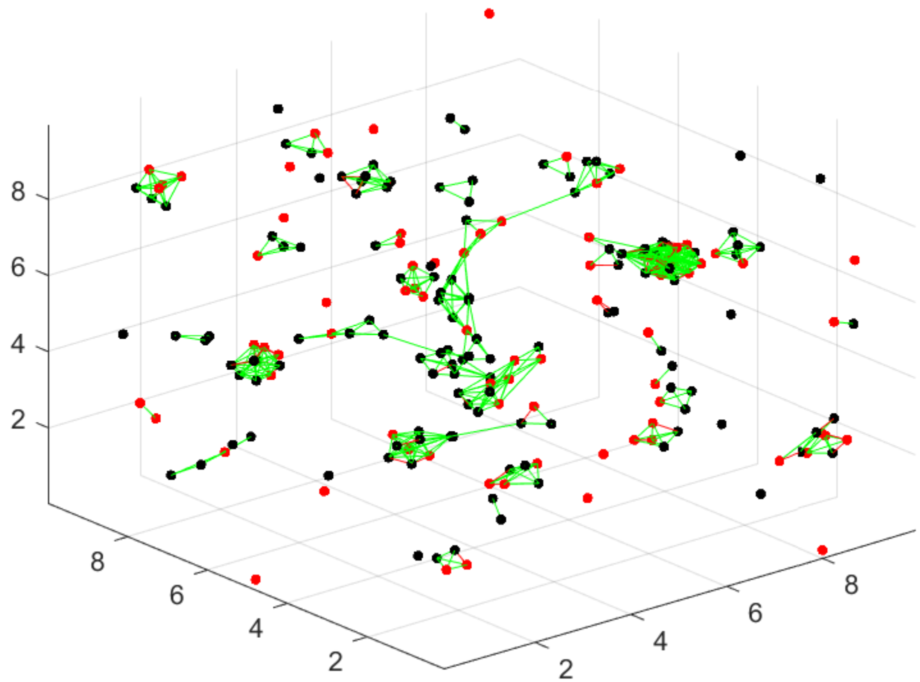
t = 50



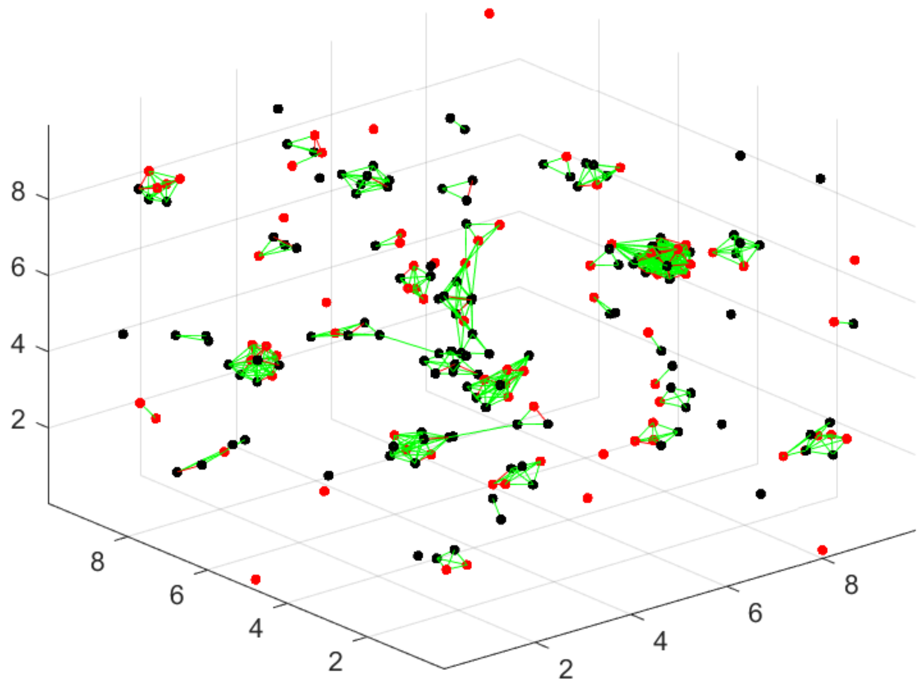

t = 60
8
6
4
2
8
6
4
2
2
4
6
8

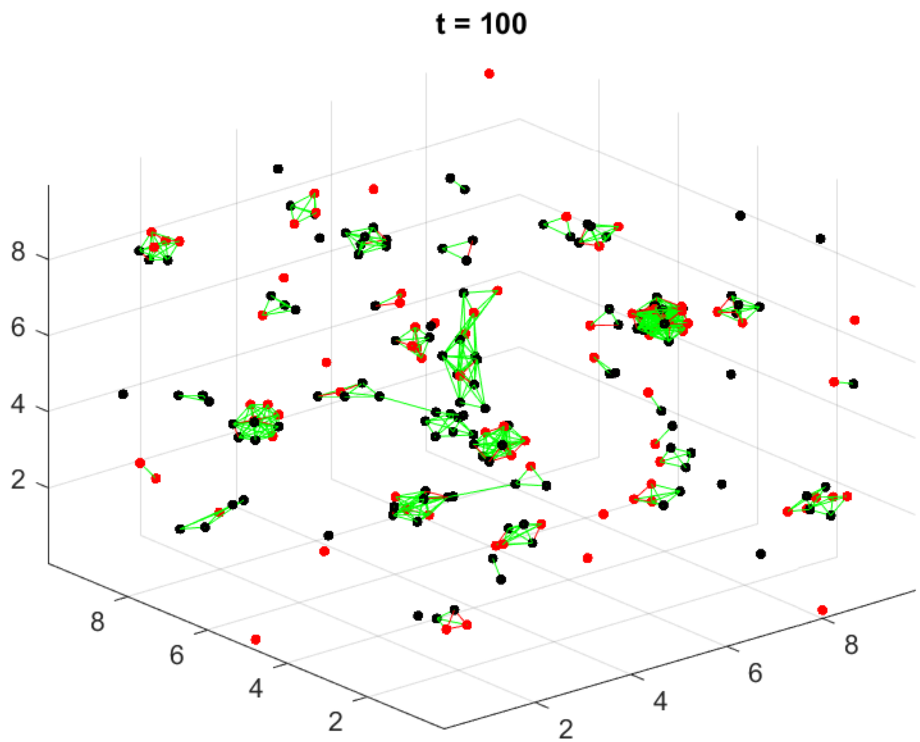

t = 70
8
6
4
2
8
6
4
2
2
4
6
8

t = 80



t = 90

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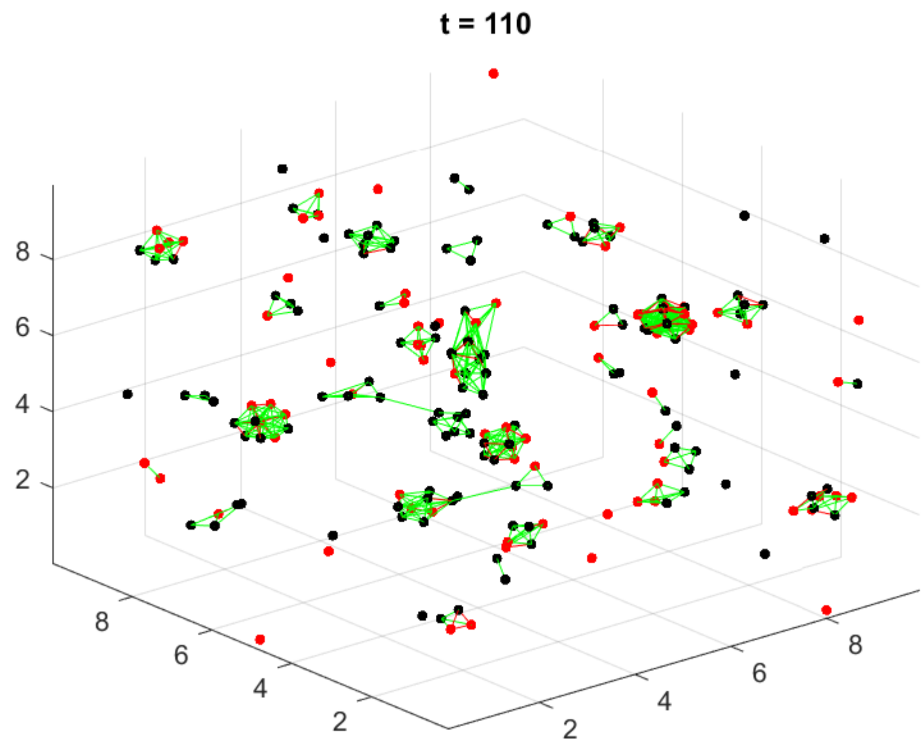
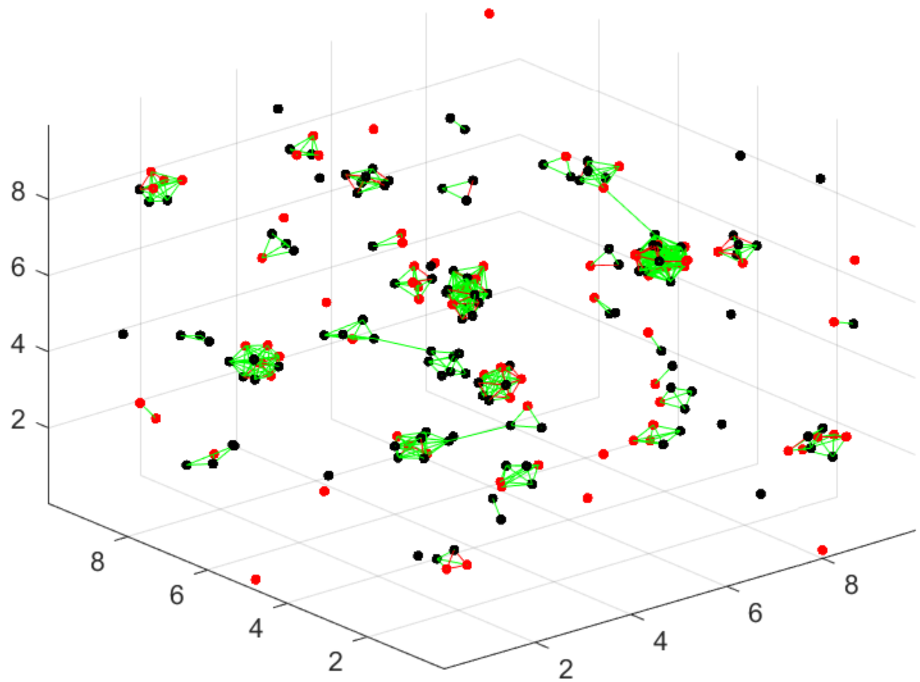
8
6
4
2
8
6
4
2
2
4
6
8

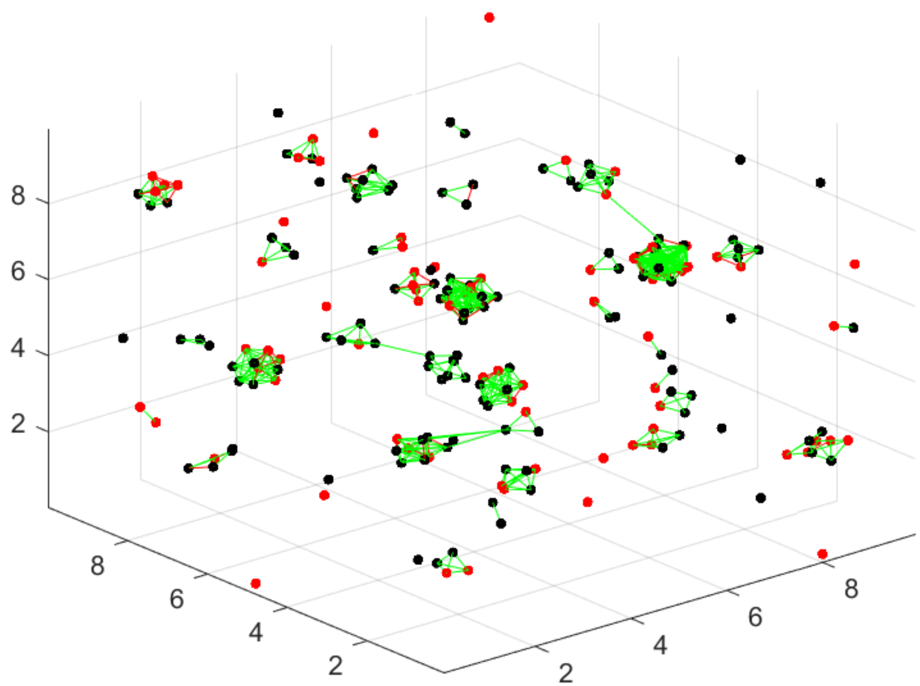


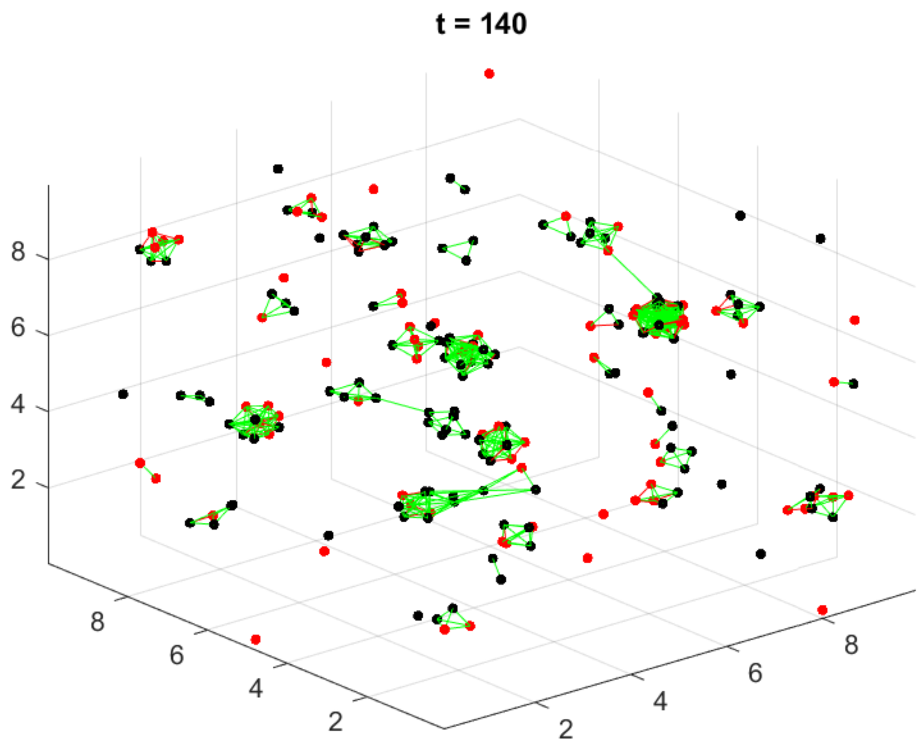
t = 110
8
6
4
2
8
6
4
2
2
4
6
8

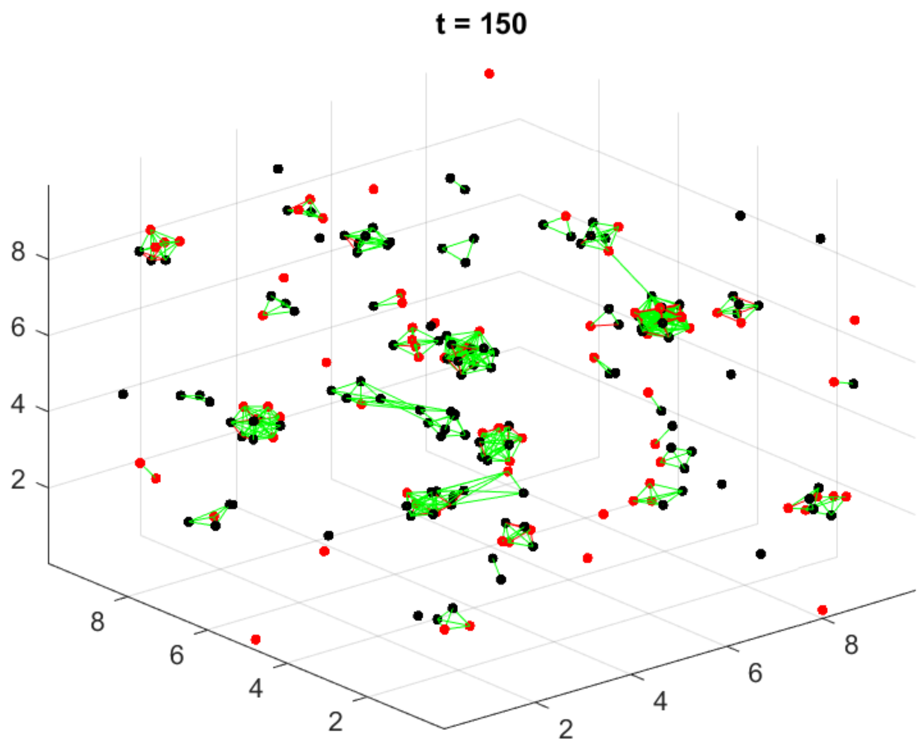
t = 120



t = 130




t = 140
8
6
4
2
8
6
4
2
2
4
6
8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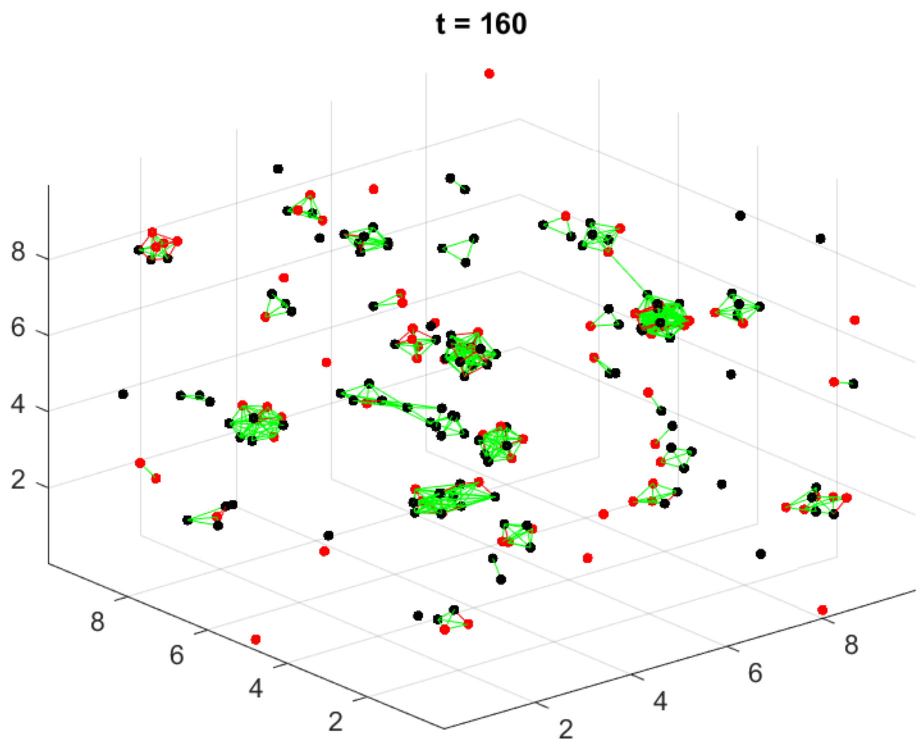
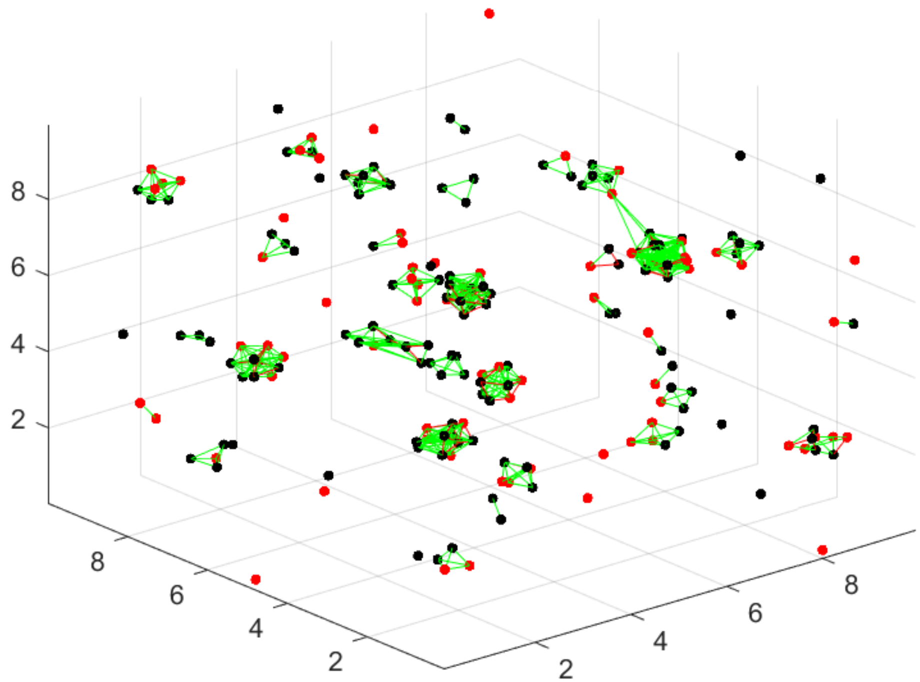
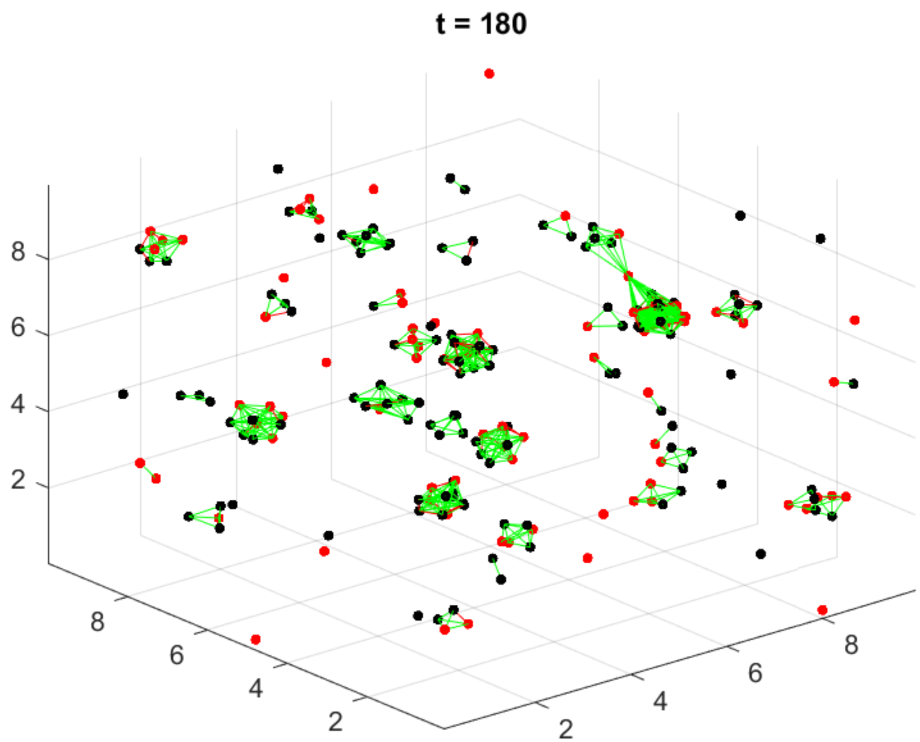
8
6
4
2
8
6
4
2
2
4
6
8

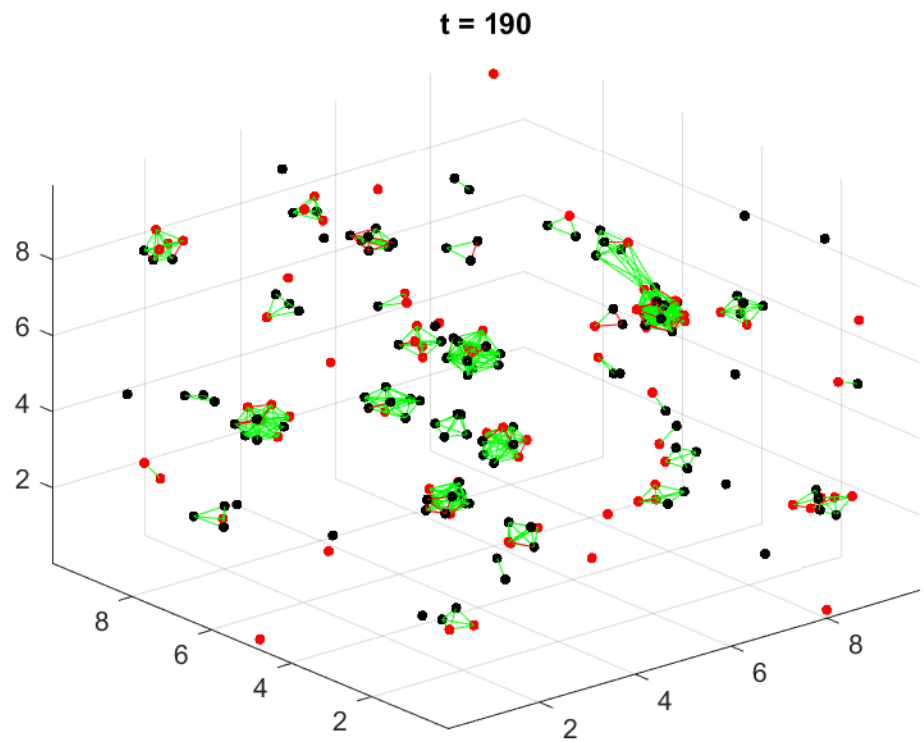

t = 160
8
6
4
2
8
6
4
2
2
4
6
8

t = 170

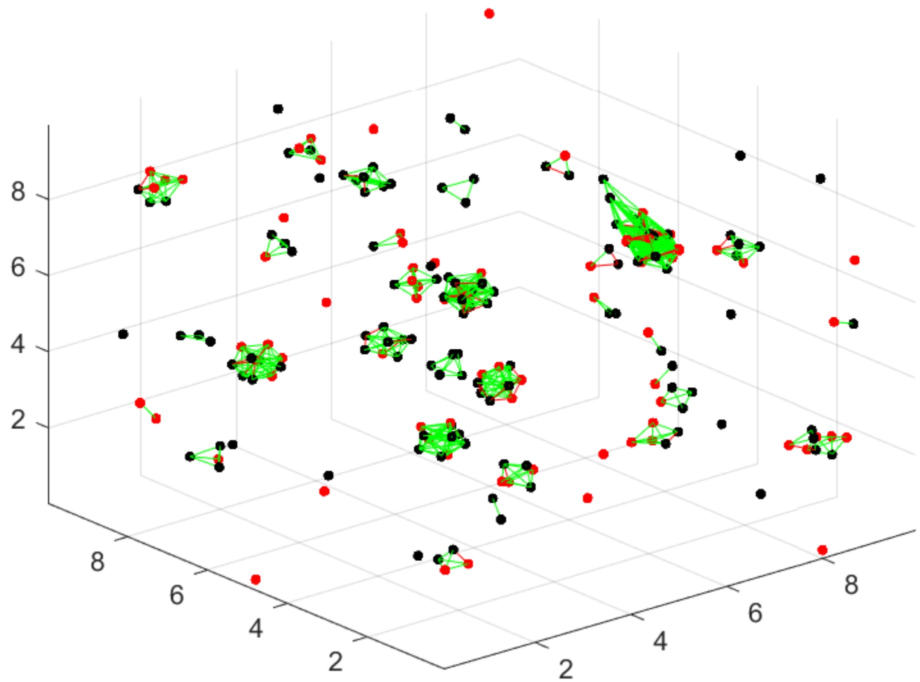


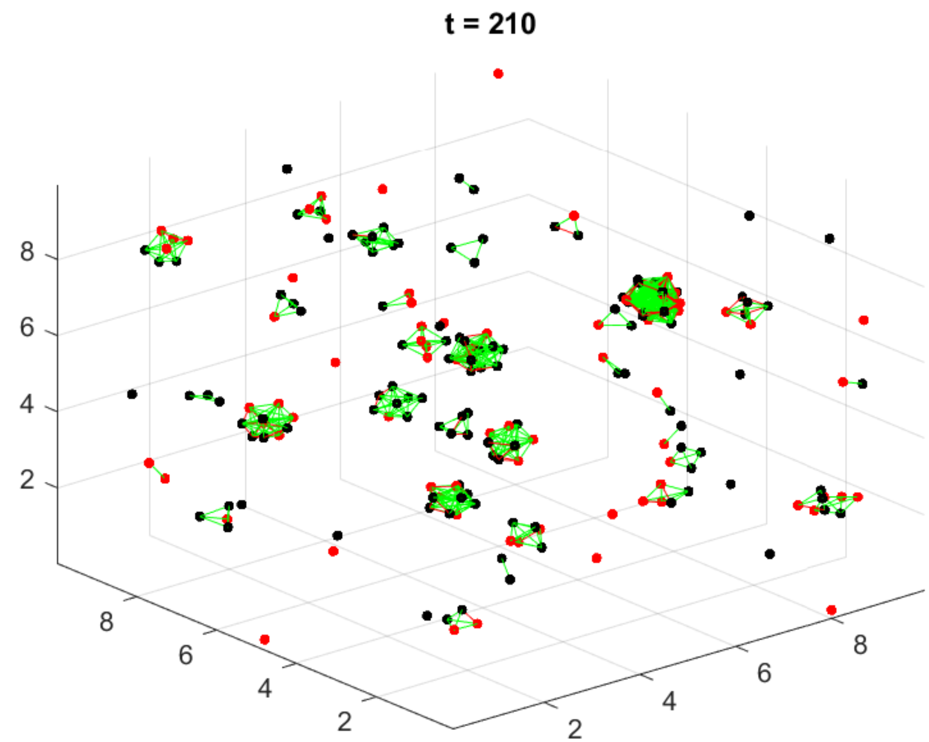


t = 180
8
6
4
2
8
6
4
2
2
4
6
8

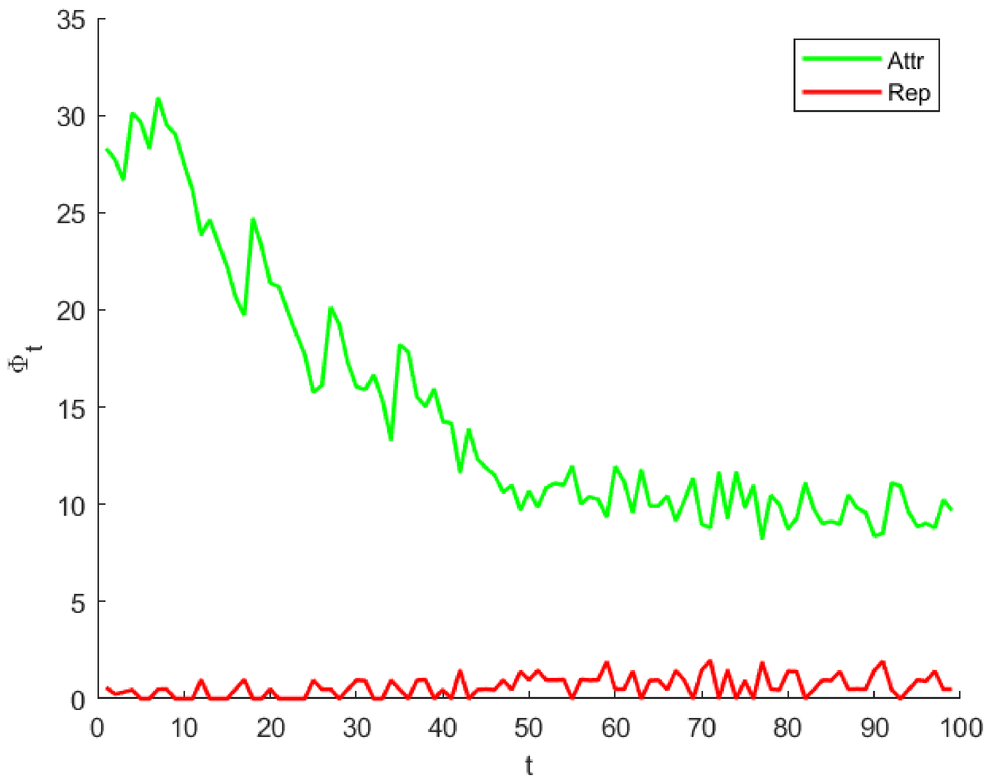

t = 190
8
6
4
2
8
6
4
2
2
4
6
8

t = 200



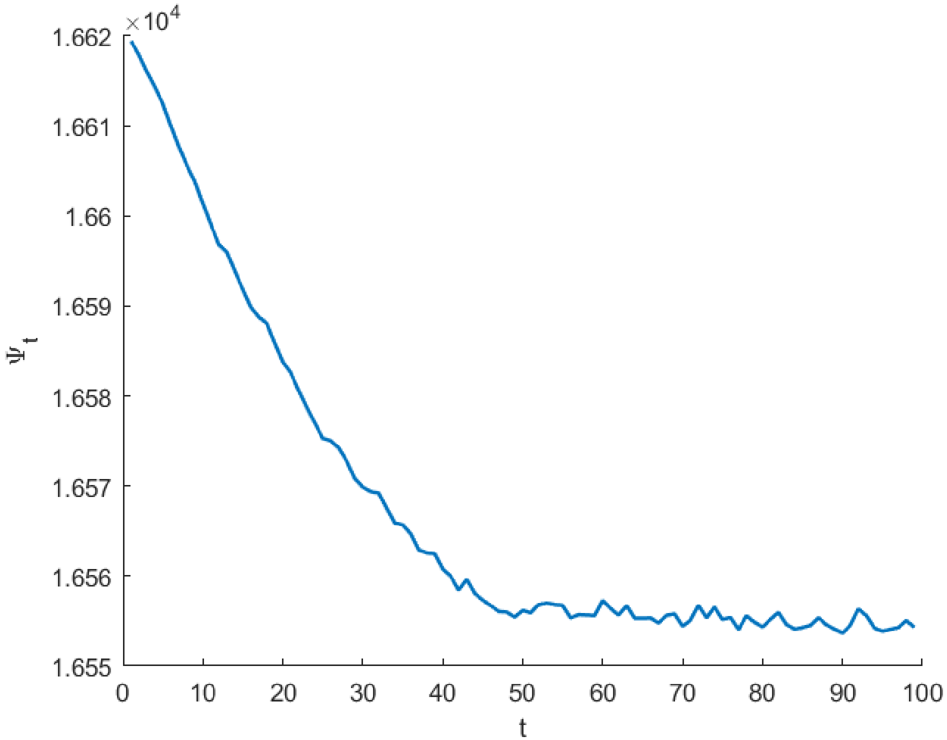

t = 210
8
6
4
2
8
6
4
2
2
4
6
8

Cluster Stabilization



Attraction and repulsion potentials change due to consensus achievement between the particles. Since the distance shortens, the attraction potential reduces and repulsion potential grows until the system reaches the state of dynamical equilibrium.

“Volume” of Interacting Particle System



Ψ Is a sum of distances between particles

Section 4

Nucleon Clustering Modelling Taking into Account the Coulomb Interaction

System Dynamics Model With Coulomb Interaction

In order to take the Coulomb interaction into account the last term is introduced:

$$x_i^{t+1} = x_i^t + z_i^t + \gamma_a \sum_{j \in N_i^t} ca_{ij}^t (x_j^t - x_i^t) - \gamma_r \sum_{j \in N_i^t} cr_{ij}^t (x_j^t - x_i^t) - \gamma_c \sum_{j \in N_i^t} cc_{ij}^t,$$

where γ_c is the Coulomb interaction gain coefficient and cc_{ij}^t is the element of a connectivity matrix Cc^t defined by parameter r_c:

$$cc_{ij}^t = \begin{cases} 1, & \text{if particles } i \text{ and } j \text{ are protons and the distance} \\ & \text{between them does not exceed certain value } r_c \\ & \text{during time interval } t \\ 0, & \text{otherwise} \end{cases}$$

Due to nonlinearity-related complications the Coulomb interaction magnitude does not depend on distance in given formulation

Simulation Model Parameters

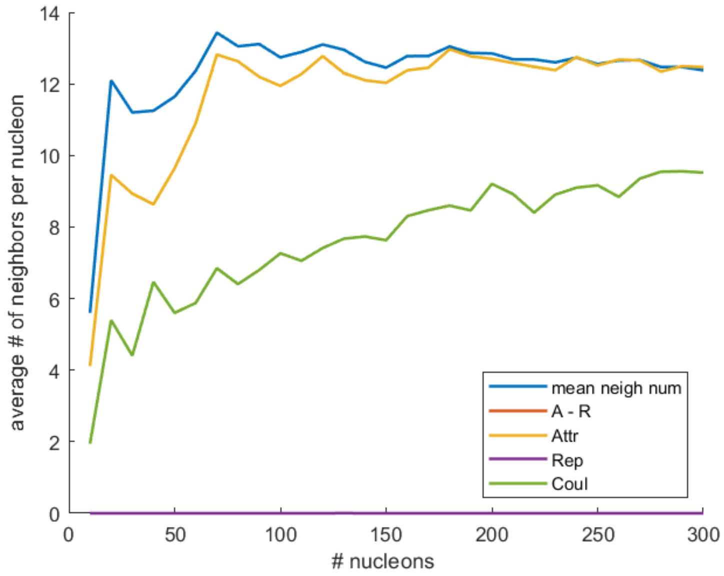
N = 252; — number of particles
Z = 82; — number of protons
T = 80; — simulation time (number of time instants)

r_attr = 1.61; — radius of particle attraction
r_rep = 1; — radius of particle repulsion
r_coul = 4; — radius of the Coulomb interaction

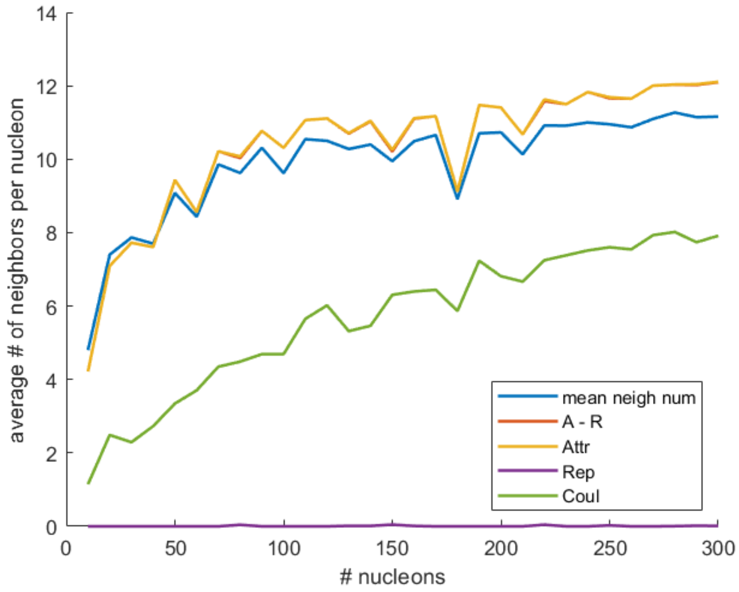
gamma_attr = 1e-3; — scale parameter of particle attraction
gamma_rep = 1e-1; — scale parameter of particle repulsion
gamma_coul = 1e-5; — scale parameter of the Coulomb interaction

initial values of particle parameter values are set randomly
Z — particle parameter values fluctuation
simulation: small constant disturbance,
$Z \in [-0.001, 0.001]$;

Average Neighbor Number per Nucleon (A = 10…300)

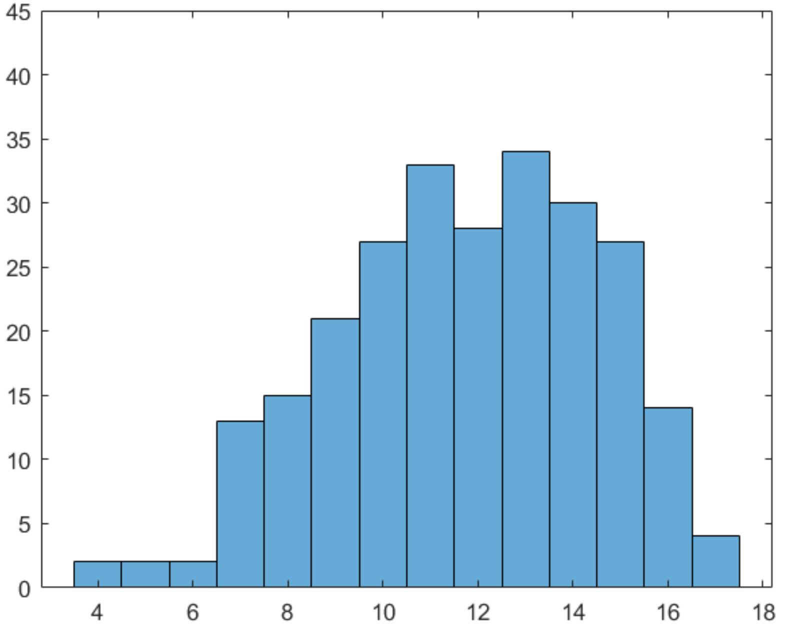


1000 iterations

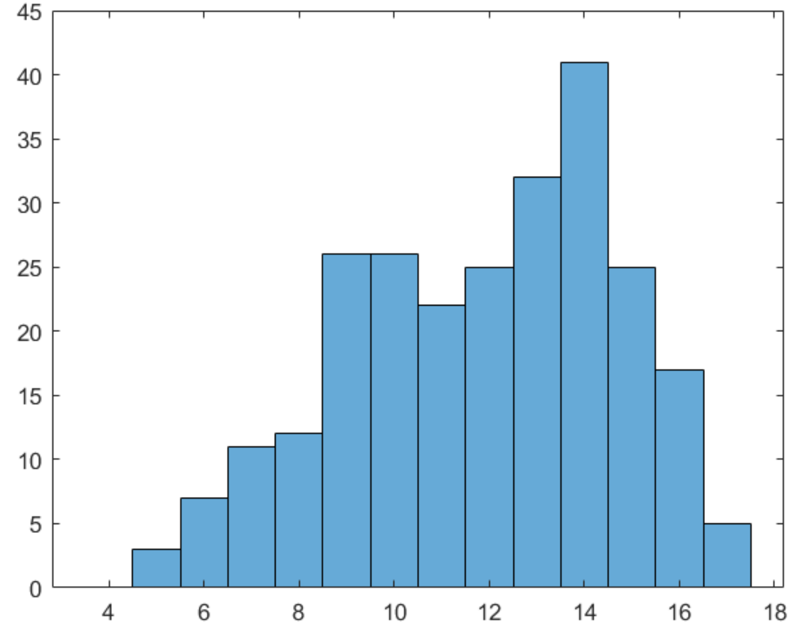


10 000 iterations

Neighbor Number Distribution

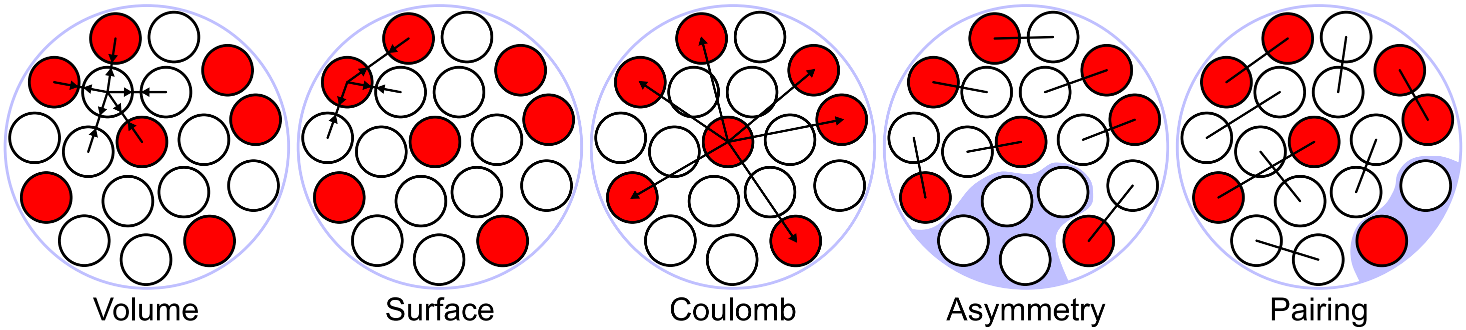


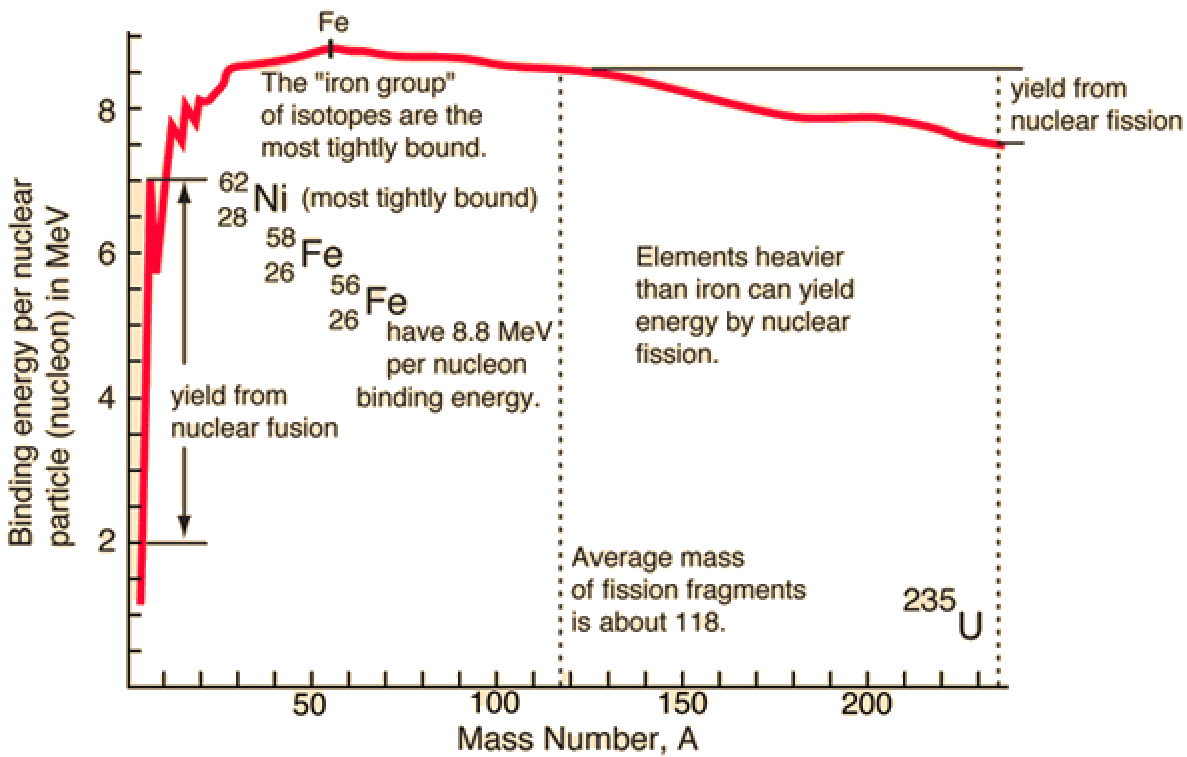
Without Coulomb interaction



With Coulomb interaction

Semi-Empirical Mass Formula





Section 5

CONCLUSION

1. The ability to model locally strong and Coulomb interactions of nucleons at the nuclear scale using a new distributed approach and the development of high-performance computing allow a better understanding of the details of the evolution of the cluster structure of heavy nuclei in fission process.

2. A novel mathematical model of nucleon clustering dynamics that explores networked multi-agent system technique was utilized. Cluster stabilization in this framework corresponds to minimizing the Laplacian potential of particles communication graph. In this approach we determine particle interaction according to the nearest neighbor rule.

3. Developed algorithm is aimed at modelling the occurrence of collective nucleon aggregation due to short-range mutual interaction taking into account the effect of coulomb interaction. Numerical simulations were performed for ^{252}Cf nucleus.

Thank you for attention!

Section 6

REFERENCES

T. Vicsek, A. Czirok, E. Ben-Jacob, I. Cohen, O. Shochet,
Novel type of phase transition in a systems of self-driven particles
Phys. Rev. Lett., Vol. 75, #6, p.1226-1229, 1995

C. Reynolds,
Flocks, herds, and schools: a sistributed behavioral model
Computer Graphics (ACM), 21(4), p. 29-34, 1987

T. Vicsek, A. Zafeiris,
Collective motion
Physics Reports 517. D, Vol. 517, #3-4, p.71, 2012

Z. Zheng, X. Lei, X. Peng,
Selective interaction and its effect on collective motion
Scientific Reports, 12(1), 8601, 2022

Lewis, Frank L., Hongwei Zhang, Kristian Hengster-Movric, Abhijit Das
Cooperative control of multi-agent systems: optimal and adaptive design approaches
Springer Science & Business Media, 2013

A. Proskurnikov, M. Cao,
Consensus in multi-agent systems
Wiley Encyclopedia of Electrical and Electronics Engineering, Wiley & Sons, 2016

A. Proskurnikov, O. Granichin,
Evolution of clusters in large-scale dynamical networks
Cybernetics and Physics, 7(3), 102-129, 2018

A. V. Unzhakova, O. N. Granichin,
Clustering and Emergent Collectivity in Multidimensional Potential Energy Surface Calculations
Exotic Nuclei: Proceedings of the International Symposium on Exotic Nuclei, pp. 351-354, 2020

A. V. Unzhakova, Y. V. Ivanskiy,
Clustering and Microscopically Separated States Formation in Fission Potential Energy Calculations
Bulletin of the Russian Academy of Sciences: Physics, 86(9), 1108-1110, 2022

Ivanskiy, Y. V., A. V. Unzhakova,
Dynamic Modeling of Clustering in Multimodal Fission of Heavy Nuclei
Bulletin of the Russian Academy of Sciences: Physics 88(8), 1267-1270, 2024