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A CLUSTERING APPROACH IN THE UrQMD TRANSPORT MODEL FOR NUCLEAR COLLISIONS AT RELATIVISTIC ENERGIES

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A method for cluster recognition from nucleon distributions generated in calculations of relativistic collisions of light particles (protons, α-particles) with nuclei in the framework of the UrQMD model is proposed. The excitation energy of the clusters which is necessary to take into account for the de-excitation of the calculated fragments was estimated from empirical considerations. The approach was applied to calculate mass distributions of fragments in $p+$Fe collisions for different proton energies and showed a good correspondence to experimental results. The software implementation of the clustering method and a visualization of cluster formation substantially facilitate applications of the proposed method.

В данной работе предложен метод выделения кластеров из распределения нуклонов, получаемого при расчетах релятивистских столкновений легких частиц (протонов, α-частиц) с ядрами в рамках модели ультрарелятивистской квантово-молекулярной динамики. Энергия возбуждения кластеров, необходимая для учета девозбуждения получаемых фрагментов, определялась из эмпирических соображений. Подход применялся для расчета массового распределения фрагментов столкновений $p+$Fe при различных энергиях протона и показал хорошее согласие с экспериментом. Программная реализация метода кластеризации и визуализация образования кластеров значительно облегчают применение предлагаемого метода.

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INTRODUCTION

Multifragmentation is a physical process occurring in high-energy collisions of nuclei or in collisions of nucleus with energetic light particles. In such types of reactions a large number of neutrons is emitted, which explains the interest to this issue in applied sciences [1]. Heavy-ion collisions, besides particle (proton, neutron, meson, hyperon, etc.) production, are accompanied by nuclear spallation with the formation of nuclear fragments. The consistent understanding of nuclear spallation over the whole energy range is a challenging task for theoretical models.

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The models that are used to describe this type of reactions can be divided into two main groups: macroscopic (statistical and hydrodynamical) and microscopic (cascade, transport) models. The main difference between cascade and transport models is that in the latter the dynamical evolution of the collision is followed microscopically in time, while in the former the potentials are taken into account only globally. The Quantum Molecular Dynamic (QMD) model [2, 3] belongs to the transport class and describes the evolution in time of the system of nucleons. The interaction is based on a nonrelativistic density-dependent Skyrme-type [4] equation of state with additional Yukawa and Coulomb potentials. The stochastic collision term gives rise to large fluctuations, compared with other transport approaches like the Boltzmann transport models, which work with the phase-space distribution. This is a very important feature when simulating the collision process including fragmentation. QMD was successfully used for calculations of isotopes production for collision energies less than 0.4 GeV [5]. There exists a version for higher energies, Ultra-relativistic Quantum Molecular Dynamic, UrQMD [6], which includes resonance excitation of nucleons and string dynamics. However, this version does not include nuclear fragmentation. Observations of multifragmentation of nuclei in collisions with protons at relativistic energies have been done in $p +$ Au collisions by the Karnaukhov group [7] in Dubna; however, they were mainly interpreted in the terms of the cascade model.

Therefore, in this paper we develop a mathematical algorithm for fragment identification in the UrQMD nucleon distribution at the final time and compare the results to the experimental data.

1. FRAGMENTATION MODEL

The first step of a UrQMD calculation is to find the positions of all nucleons at the initial stage of reaction. Projectile and target are modeled according to the Fermi-gas ansatz: it means that the initial momenta of the nucleons are randomly chosen between 0 and the local Thomas–Fermi momentum. The nucleons are represented by Gaussian shaped density distributions: its binding energy should correspond to the value given by the Bethe–Weizsäcker formula and its radius should yield the following mass dependence: $R(A) = r_0 A^{1/3}$, where A is the mass number and the parameter r_0 is a function of the nuclear matter ground state density ρ_0 [6].

An example of the nucleon distribution for the reaction $p +$ Fe (4 GeV/nucleon) at $t = 0$ is shown in Fig. 1 (left). Here the collision partners are already boosted to the initial velocity, such that the nucleus is relativistically contracted. Then the time evolution of the spatial distribution of nucleons and mesons (pions, kaons, etc.) is traced. For the propagation of the nucleon coordinates, the set of coupled discretized Hamiltonian equations is solved:

$$\begin{aligned} \mathbf{p}_i(t + \Delta t) &= \mathbf{p}_i(t) - \Delta t \boldsymbol{\nabla}_r U_i([r_j, p_j]), \\ \mathbf{r}_i(t + \Delta t) &= \mathbf{r}_i(t) + \Delta t \mathbf{p}_i(t)/m. \end{aligned} \tag{1}$$

Here $U_i([r_j, p_j])$ is the potential acting on particle i, which depends on the coordinates and momenta of the other particles via the two-body interactions. In between the time steps the collision term is evaluated stochastically taking into account the two-nucleon cross section. One can follow the changes of nucleon distributions in time from one time step to another.

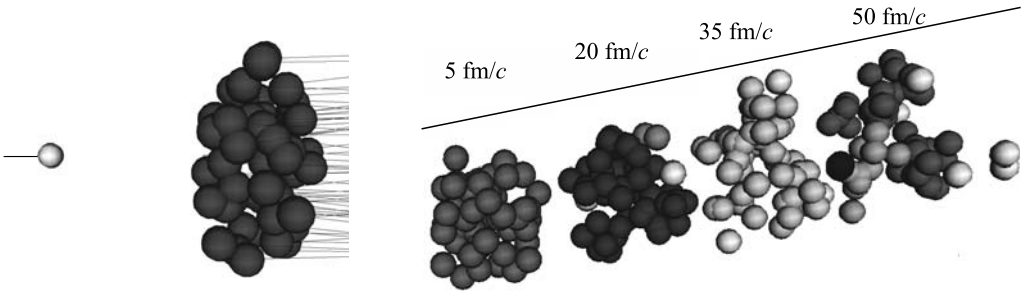

Fig. 1. Example of the time evolution for the reaction p+Fe (4 GeV/nucleon): left — initial distribution at $t = 0$; right — distribution at time steps $t = 5$, 20, 35, and 50

The example of time evolution is represented in Fig. 1 (right) for the same reaction. One can see that, according to the UrQMD results, the energy deposited in the nucleus as a result of the collision is not distributed uniformly and the nucleus does not have time to equilibrate. The reaction mechanism looks like a knockout reaction for the fast nucleon and a fragmentation of the highly excited target residue.

The next step is to identify the nuclear fragments at the final time of the reaction and determine their kinetic energies, masses, and binding energies. At the last stage the de-excitation of the excited fragments is calculated.

2. CLUSTER FORMATION

As a result of the UrQMD calculation, we obtain a table with the positions, momenta, and other characteristics of nucleons and other particles produced in the reaction for the chosen time steps. To find the clusters in the final distribution, we assume that a group of A nucleons forms a fragment when the following conditions are satisfied:

1) The nucleons of the group are close to each other, while nucleons which do not belong to the fragment are away from it.

2) The group radius, i.e., the maximal distance of a particle from the center of mass, is not greater than $L_k^{\max} = 1.5A^{1/3}$, where $A = N(S_k)$ is the number of nucleons in group k.

In addition, we assume that with condition (2) it is possible to demarcate realistic fragments heuristically. From the many existing clustering algorithms [9] the single linkage agglomerative [8] was chosen, because it was empirically proved that it was the best in comparison with the other clustering algorithms.

The mathematical method for cluster recognition, implemented in the UrQMD code, proceeds as follows. For each nucleon i a vector x_i of Euclidean space R^3 is defined, which is used as a base for clustering. The clustering result is a set $S = \{S_j\}$ of disjoint sets, which are clusters $S_j \subset V$ of nucleons $V = 1, 2, \ldots, n$ in the current time frame (where n is the number of fragments to be clusterized). The clustering method is then divided into 3 steps: (1) application of the single linkage cut to the nucleons; (2) singleton clusters removal; (3) fragment postfiltering.

1. Single linkage cut. The single linkage cut can be described by the following definition:

a) Let $G = \langle V, E\rangle$ be a graph on nucleons V, where E is a set of edges defined as $E = \{(s,t) \mid\mid\mid x_s - x_t \mid\mid < d_{\max}\}, s \in V, t \in V$.

b) Then the set of sets $S = \{S_j\}$ is a single linkage cut, if:

i) there is a one-to-one mapping between the connected components in G and S;

ii) each set S_j is a set of nucleons in a corresponding connected component.

2. Singleton clusters removal. The algorithm puts nucleons that are away from any other cluster into distinct clusters which are called singletons. These singletons should be removed (as they are not fragments). The removal is done in the following manner: $S <= \{S_j : N(S_j) > 1\}$.

Postfiltering. It is clear that the algorithm can form clusters which are stretched in coordinate space, while fragments should be compact in space according to the condition (2). In order to meet this condition, we perform postfiltering on such fragments, removing distant nucleons. The postfiltering algorithm is as follows. For each cluster S_k:

a) find a center of mass $\mu_k = M[x_j], j \in S_k$;

b) erase from S_k nucleons which are farther from the center than $L_k^{\max}$: $S_k <= \{i \mid\mid\mid x_i - \mu_k \mid\mid \geqslant L_k^{\max}\}$.

Thus, $L_k^{\max}$ has the meaning of the fragment radius.

3. RESULTS

The cluster formation method discussed above was applied to calculate nuclear fragmentation in the reaction of protons with iron, p + Fe, at proton energies of 1.5 and 1.0 GeV per nucleon. UrQMD calculations were performed, and the clusterization program allowed us to obtain the distribution of masses of the produced fragments at different time steps. It was observed that the smallest time step for the fragmentation process is about 50 fm/*c*. The produced fragments are still in excited states. The excitation energies were estimated

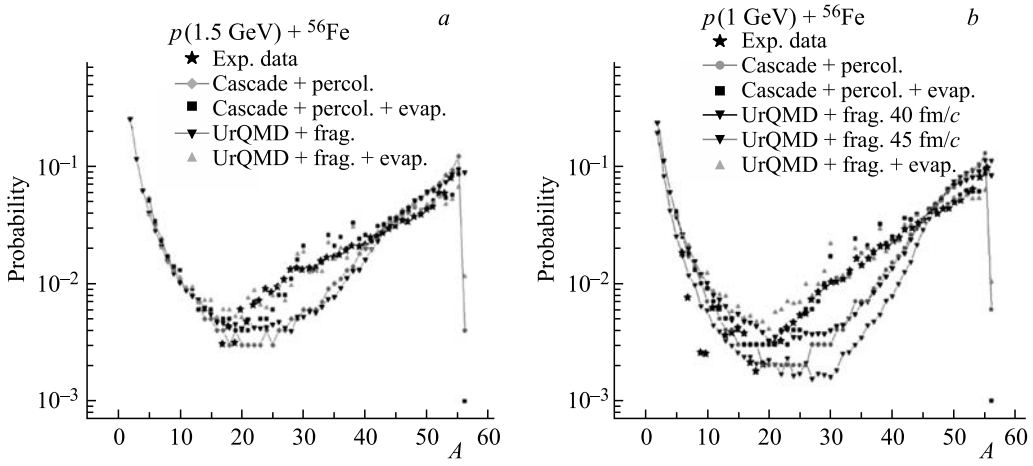

Fig. 2. Mass distributions of fragments in p + Fe for different proton energies: *a*) 1.5 GeV; *b*) 1.0 GeV [10]

from the energy conservation law and divided between fragments in proportion to their mass. For comparison calculations were also done in the cascade + percolation model that allows one to take into account the excitation energy of produced clusters (see [10] and references therein). The obtained mass distributions for both methods are shown in Fig. 2 and compared with the experimental results [11]. One can see that the results of both calculations are much more different from the experimental data, if we deal with primary excited nuclei, but fit experimental data reasonably well after evaporation is taken into account.

CONCLUDING REMARKS

The method describing multifragmentation reactions for energies greater than 0.4 GeV/nucleon with the UrQMD transport model is developed. It uses the single linkage clustering approach with special postfiltering, which allows one to identify fragments in the final nucleon distribution. The comparison with experimental data shows that the approach is quite promising for physical applications. The software implementation of the clustering method and the visualization of the cluster formations are done in a user-friendly framework, which substantially facilitates the applications of this method.

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