In this contribution, effectiveness of parallel SFF-PFUMILI calculations is demonstrated at the cluster HybriLIT, new results of SANS analysis of ULV structure are presented.

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Molecular-Dynamic Modeling of Long-Range Effect in Metals Exposed to Nanoclusters

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Irradiation of metal targets by pulsed ion beams can be approximately modeled as irradiation by a sequence of nanoclusters, and in this case the problem can be considered in frame of the molecular dynamics method.

At present, for the application of molecular dynamics methods, there are ready-made software packages (LAMMPS, NAMD, etc.). In this work, the simulation was carried out using the LAMMPS package installed on the HybriLit cluster, which was modified in accordance with the task of modeling the simultaneous interaction of several nanoclusters with the target.

The simulation was carried out as follows. Within the molecular dynamics approach, we solve the problem of irradiating a metal target with several nanoclusters with different energies. Then, using the solution obtained, we calculate temperature profiles of the target as a function of time. To do this, the target material is divided into cells and in each cell we calculate the temperature for each step in time. The computational domain was a parallelepiped $22 \times 22 \times 16$ nm.

The present paper differs from previous works in that the metal target is irradiated simultaneously by two nanoclusters, the interaction regions of which with the target surface are at a certain distance (2–3 nm). Since the wave transfer of heat propagates diagonally, this results in the fusion of moving regions with a high temperature in the depth of the target. The temperature in the fusion region sharply rises, exceeding the melting temperature of the target, which can lead to structural changes in the target. It is numerically determined that this region is located at the depth of the target, exceeding the depth of penetration of the cluster. This result can be applied to explain the effect of long-range action.

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A Wigner Potential Decomposition in the Signed-Particle Monte Carlo Approach

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The description of the electron evolution governed by an electric potential in terms of a phase space formulation of quantum mechanics is provided by the Wigner equation. The latter comprises of a force-less Liouville operator, which is associated with particles moving over Newtonian trajectories, and a Wigner potential operator associated with generation of positive and

negative particles. These concepts can be combined to develop stochastic algorithms for solving the Wigner equation, consolidated by the so-called Signed Particle approach. A peculiarity of the approach is that signed particles reside on a grid in the momentum space.

We investigate the option to split the Wigner potential into two parts and to approximate one of them by a classical force term. The purpose is two-fold. First, we search for ways to simplify the numerical complexity involved in the simulation of the Wigner equation. Second, this term offers a way to a self-consistent coupling of the Wigner and the Poisson equation. Therefore, the physical potential is split into a slowly-varying classical component and a rapidly-varying quantum component through the definition of an ideal low-pass filter with a cut-off wavenumber.

The particles in the signed-particle method experience a force through the classical component of the potential. A cellular automaton algorithm is used to update the discrete momentum of the accelerated particles. Furthermore, the quantum mechanical component which vanishes at infinity and has a smooth Fourier transform is used to efficiently calculate the reduced Wigner potential and the corresponding generation processes. Therefore, the quantum character of carrier transport is coupled to the classical evolution of particles in the proposed approach. For illustration purposes, the evolutions of minimum uncertainty wavepackets (density) in a two-dimensional region are presented for various cut-off wavelengths and potential profiles.

Interdisciplinary Aspects of the Classification Studies

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The purpose of this paper is an illustration of the broad range of applicability of the classification studies in many diverse areas of science. In particular, in our previous works we have designed several new classification methods in computational biology, physics, chemistry, astronomy. In biology, the classified objects are the biological sequences. In the present work, details of one of the methods, called by us 2D-Dynamic Representation of DNA/RNA sequences, are described. The main idea of this approach is borrowed from the classical dynamics. The biological sequence is represented by a 2D-dynamic graph treated as a rigid body. The numerical values, called descriptors, form a basis for the creation of highly accurate classification maps. The maps facilitate the detection of some unknown properties of the sequences.

In the present work, we also show the usefulness of the classification studies in the health sciences. For this purpose, we perform numerical analysis of the data collected from 449 individuals and evaluated according to the World Health Organization Quality of Life-BREF questionnaire. This is a standard questionnaire used in many countries in the studies on the quality of life. The graphical representation of the results we perform using the correspondence analysis. As a consequence, we obtain classification maps in which the objects under consideration are groups of the individuals, and their answers to the questions. The classification of the groups of individuals is then performed by an analysis of the distribution of clusters in the classification maps. In the present work, we study the significance of gender on the results.