

ACTIVITIES RELATED TO SCIENTIFIC VISUALIZATION AT NATIONAL RESEARCH NUCLEAR UNIVERSITY "MEPHI", MOSCOW, RUSSIA: RESEARCH, EDUCATION AND PUBLICATIONS

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In this paper we present the results of scientific visualization research as a joint project of the NRNU MEPhI (Moscow, Russia) and the National Centre for Computer Animation, Bournemouth University (Bournemouth, United Kingdom). We consider scientific visualization as a modern computer-based method of data analysis. The essence of this method is to establish the correspondence between the analyzed initial data and their static or dynamic graphical interpretation analyzed visually. The results of the analysis of graphical data are interpreted in terms of both the initial data and the reality behind it. The method of scientific visualization as a method of scientific data analysis is a method of spatial modeling of those data. It allows for utilizing enormous potential abilities of a researcher and their spatial imaginary thinking in the process of data analysis. In the general case, the process of data analysis using the method of scientific visualization can be quite complex, iterative and interactive. This article is devoted to results of research and educational projects. These projects are quite different and multidisciplinary. The goals of the data analysis can be different as well. As a result, in most cases significantly different graphical representations can be involved.

Keywords: scientific visualization, data analysis, multidimensional analysis, method of scientific visualization, multisensory analysis, research and educational projects

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1. Introduction

In this report, we would like to present the results of scientific visualization research as a joint project of the NRNU MEPhI (Moscow, Russia) and the National Centre for Computer Animation, Bournemouth University (Bournemouth, United Kingdom). We consider scientific visualization as a modern computer-based method of data analysis [1]. The essence of this method is to establish the correspondence between the analyzed initial data and their static or dynamic graphical interpretation analyzed visually. The results of the analysis of graphical data are interpreted in terms of both the initial data and the reality behind it (Fig. 1).

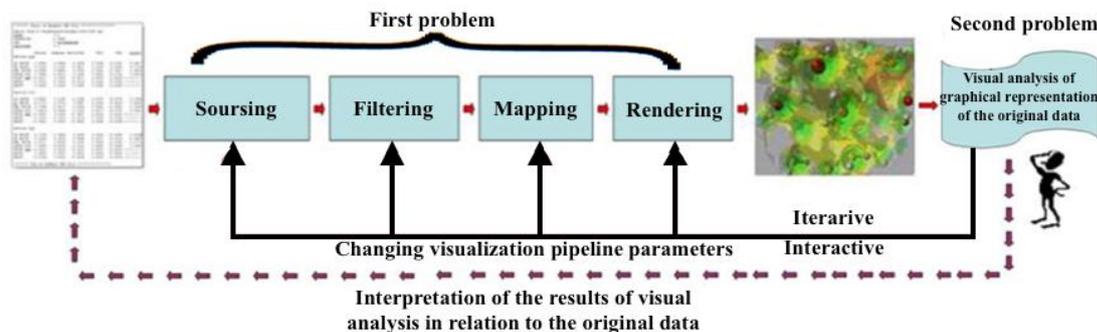


Figure 1. Scientific visualization method of data analysis

What does actually visual analysis of graphical data representation constitute? It is a matter of principle to understand that qualitative visual analysis consists of the analysis of the spatial interpretation correspond to the initial data. This means that the obtained graphical images serve just as means for natural and convenient representation of the spatial interpretation to the researcher for analysis. It is followed by the interpretation of the results in terms of the initial scientific data. Thus, the method of scientific visualization as a method of scientific data analysis is a method of spatial modeling of those data. It allows for utilizing enormous potential abilities of a researcher and their spatial imaginary thinking in the process of data analysis. As the result of solving these problems, some conclusions are made by the researcher regarding the spatial scene. As mentioned above, these conclusions are then interpreted in terms of initial data. Thus conclusions are formed regarding the object of study. In the general case, the process of data analysis using the method of scientific visualization can be quite complex, iterative and interactive.

The works of mention above joint project in scientific visualization field are carried out in three related directions:

- Scientific Visualization of Physics Research,
- Scientific Visualization in Physics Education,
- “Scientific Visualization” Journal Publication.

We would like to underline that in all these directions we consider Scientific Visualization as a method of data analysis.

2. Scientific Visualization in Physics Research

Nowadays mentioned above scientific visualization method is widely used by various physics research groups at NRNU “MEPhI” [2]. The research is carried out by physics departments, educational and scientific laboratory “Scientific Visualization” of NRNU MEPhI and NCCA of the Bournemouth University.

A complex of software tools on base of different 3D modelling and visualization programs (3DS Max[3], HyperFun[4], Jmol applet [5], VTK[6], Cortona3D[7]) was created as a result of this collaboration. Interaction of different software components is shown in Fig. 2.

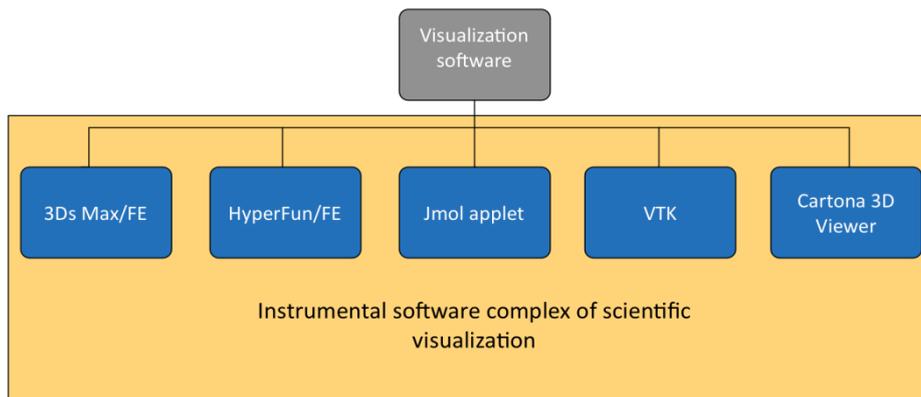


Figure 2. Interaction of the visualization software and the complex

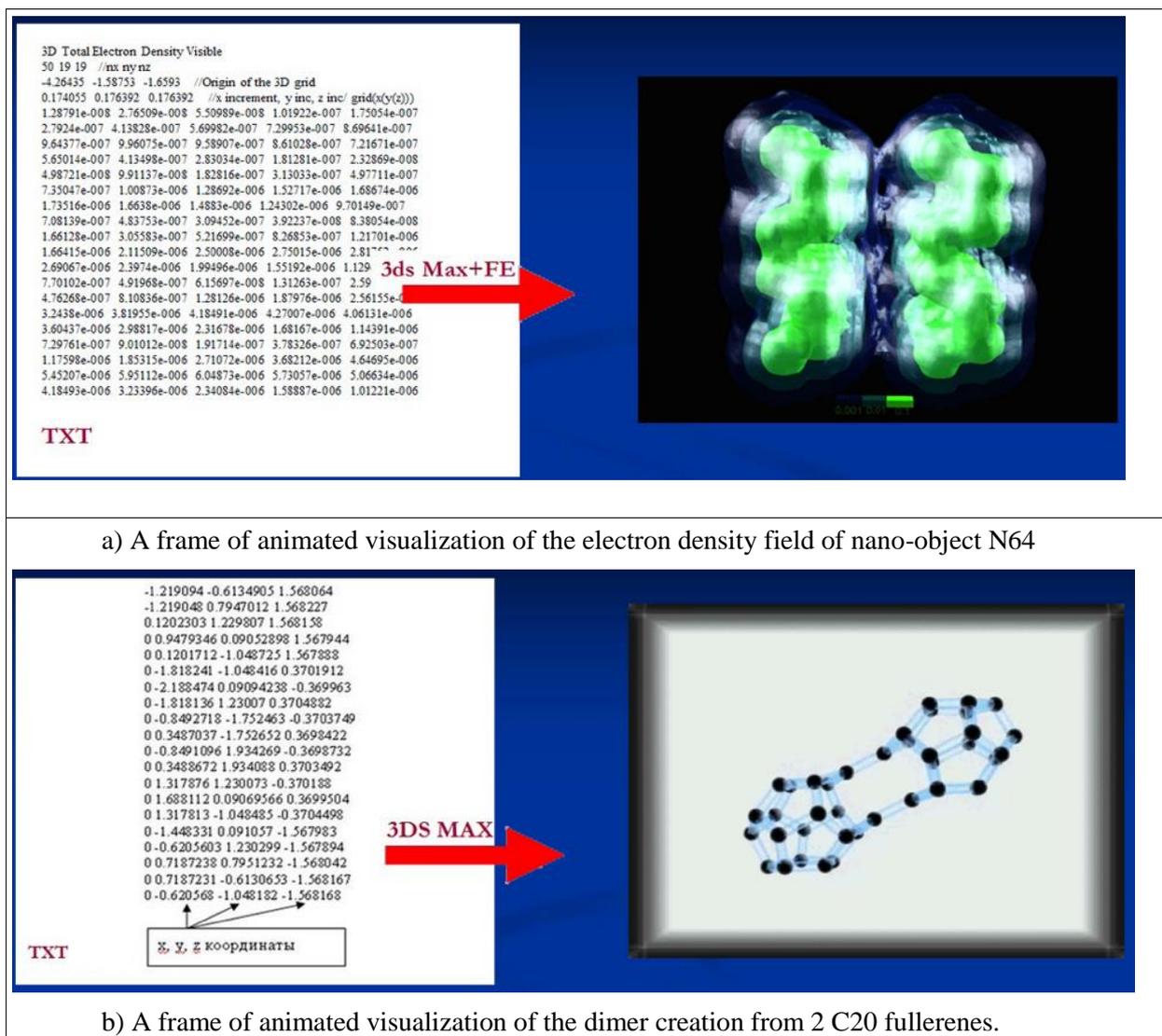


Figure 3. Examples of the nanostructure visualization

The main purpose of these programs is to provide researchers of joint university groups with flexible research tools in their studies of such data as nanostructures and in multidimensional scalar field visual analysis. As already noted, the research is closely connected to teaching. These tools were designed to be used in research and education with development of appropriate e-learning tools including multimedia courses, virtual laboratory works and other materials. Some of these educational projects will be described below.

Let's consider some examples of the results obtained on base of the software complex.

2.1. 3D Studio Max

On Fig. 3 we presented an example visualization results of two application programs, written on the basis of 3D Studio Max (3ds MAX). Noted that most of those programs were created as a result of collaboration of the Scientific Visualization Laboratory with researchers from physics departments of NRNU. The software is written in MaxScript and uses components of 3ds Max with specially written plugins for scientific data visualization. The input data of the visualization software were presented in specific data formats used by NRNU researchers. Widely used nanostructure descriptive formats XYZ, HIN, OUT, and MOL files. These files are output of some nanostructure computer modelling software (HyperChem, Gamess [8, 9]) as well as applications written by physicists of NRNU MEPhI [10].

2.2. Nanomodeller program

The “Nanomodeller” program was created as a result of collaboration of the Scientific Visualization Laboratory with researchers from physics departments NRNU and researchers from the Photochemistry Center of the Russian Academy of Sciences. It was developed and used by researchers in their work on nanostructures modelling visualization and editing molecular structures procedures [11]. An example of Nanomodeller functional procedure is presented on Fig.4.

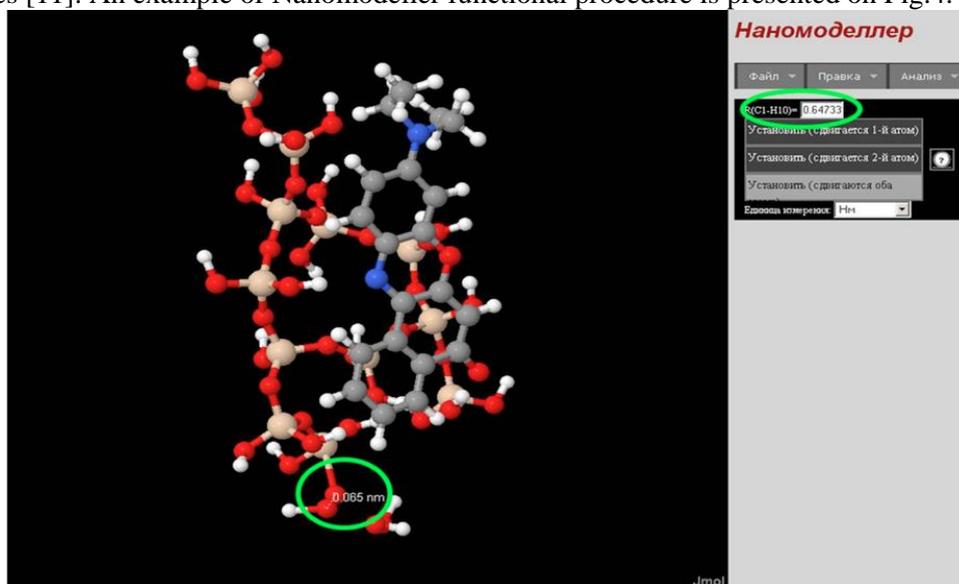


Figure 4. Functional procedure in Nanomodeller – changing distance between two atoms

2.3. HyperFun+VTK project

HyperFun [4] and VTK [6] integration based project is a result of collaboration of the Scientific Visualization Laboratory and NCCA of Bournemouth University. The results of this collaboration are not only computer software program, but theoretical studies in modern scientific visualization field trends as multidimensional and multisensory visualization [12, 18] and laboratory works, that will be described in the next section.

Here, particular attention is paid to geometric model involved in scientific visualization to be compact, precise and with unlimited complexity. The model is based on a constructive approach to the creation of the function evaluation procedures of geometric shapes called the Function Representation (FRep) [13]. Software program HyperFun is used to work with FRep modelling.

The software is mainly oriented to visualization of multidimensional scalar fields as results of computer simulation. The studied scalar fields were given as functions of several variables defined on domains represented as geometric objects that also could be defined by functions of several variables. The visualization was made through the Visualization Toolkit (VTK) [6] based interface for HyperFun [4]. Example of dynamic scalar field visualization is presented on Figs. 5.

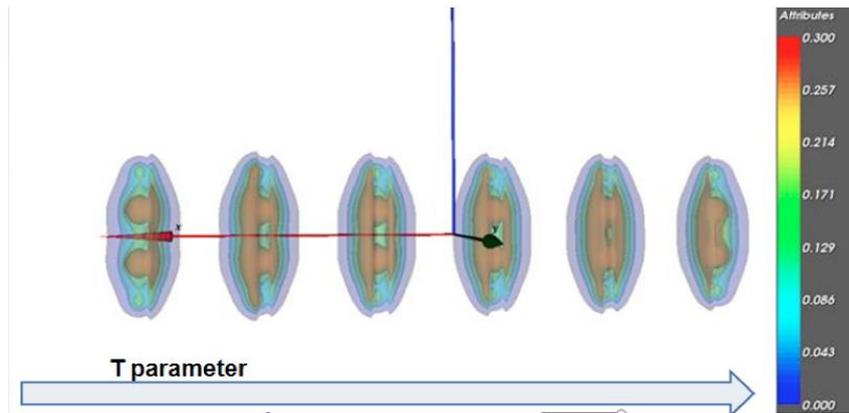


Figure 5. Example of dynamic scalar field visualization. Visualization of dynamic electron density field of C2H2 molecule

Examples of multisensory visualization of two scalar fields (electron density and electrostatic potential fields of NCH molecule) are presented on Fig. 6: the collection of semi-transparent isosurfaces, colored with values of second field and with several positions of the point sound source (red sphere).

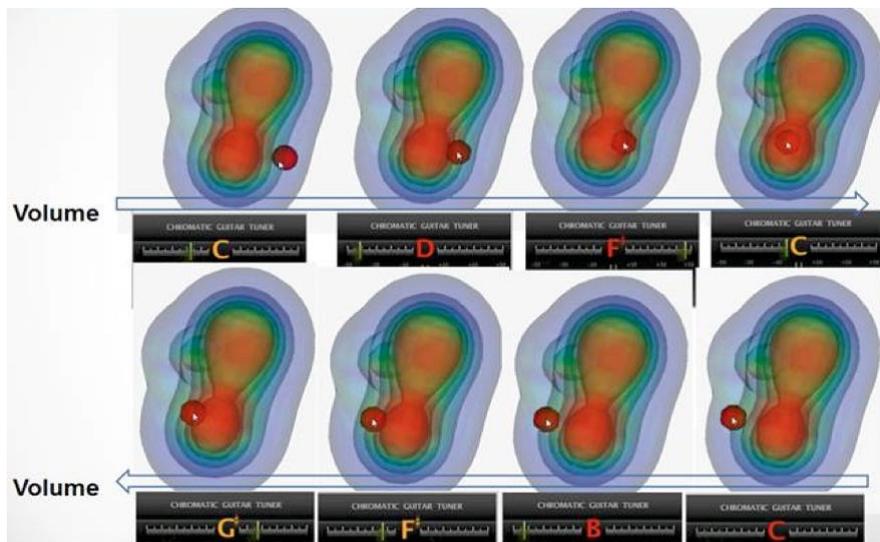


Figure 6. Screenshots of the interactive visual-auditory display of two scalar fields

The results of the visual and auditory rendering of the spatial scene are the following:

- a graphical image of projections of semi-transparent colored isosurfaces on a graphical terminal;
- the point sound source represented by the red sphere with the sound source located in its center. Its location is specified interactively by the user;
- sound wave generated by a sound terminal with the frequency corresponding to the value of first field (electron density field) in point of location of the point sound source and perceived by the user as a specific sound tone.

3. Scientific Visualization in Physics Education

Nowadays, it is especially important for students in physics to have skills in computer modelling of physical objects and processes that can be very helpful in their research work. As scientific visualization tools are widely used for analysis of computer modelling results, students in physics are often taught to visualize results of computer modelling as well [15]. The described above HyperFun+VTK software tool was used as a scientific visualization tool for analysis of various physical objects and processes that are the results of computer modelling in educational and research

studies of students of physics departments at the NRNU "MEPhI". Laboratory practical materials were created in support. Most often, the studied results of computer modelling are physical scalar fields. Students are taught to consider different static and dynamic spatial images of computer modeled scalar fields in the process of their analysis by means of scientific visualization. Some of the results of scientific visualization problems solved by students as a part of their laboratory work are presented on Fig.7.

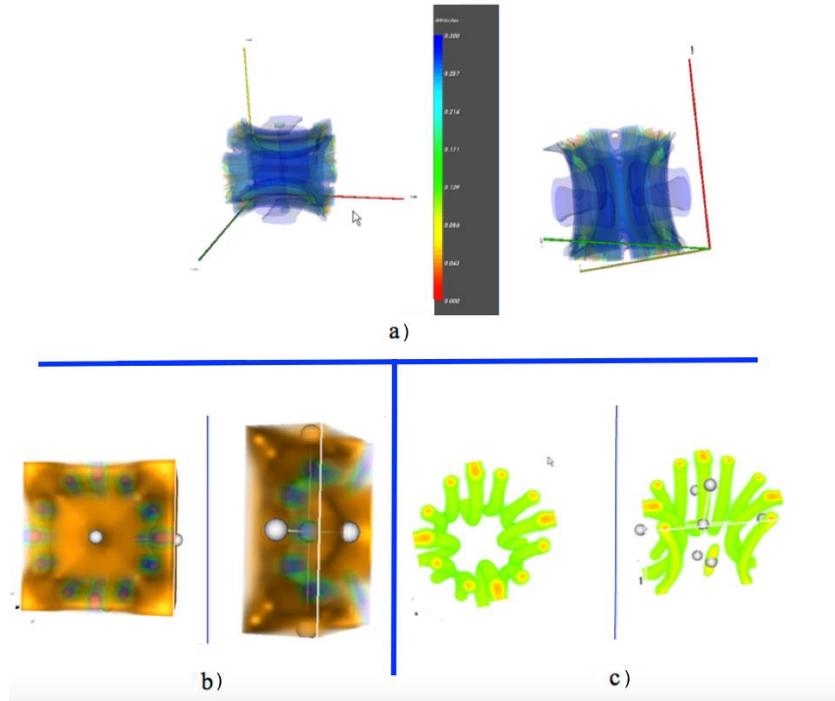


Figure 7. Scientific visualization example of the order-parameter field for the second type superconductor (Abrikosov vortices)

Different approaches to scalar field visualization:

- a) isosurfaces;
- b) volume visualization with the scalar field defined on a rectangular domain;
- c) scalar field on a complex domain defined by one of the field's isosurfaces.

The field's domain can be interactively cross-sectioned by the user with planes controlled by white handles.

One more example is "The Scientific Visualization" course, which is taught to PhD students in physics at the NRNU "MEPhI" [16, 17]. This course was developed by the Scientific Visualization Laboratory with support of physics departments and the NCCA, Bournemouth University, UK. The purpose of this course is studying theoretical principles of scientific visualization and acquisition of practical skills in development of scientific visualization software. In general, the course aims to develop the students' spatial creative thinking while solving problems of scientific data analysis. So, this course teaches students to consider and manipulate the corresponding spatial images, to make their visual analysis and to interpret the analysis results in terms of the application area.

The course includes the following three sections: scientific visualization concepts and capabilities, scientific visualization tools, and scientific visualization applications. All three sections use the mentioned above software as an example. In the practical part of the course students write software programs on the basis of the software complex mentioned in the Introduction.

4. “Scientific Visualization” Journal Publication

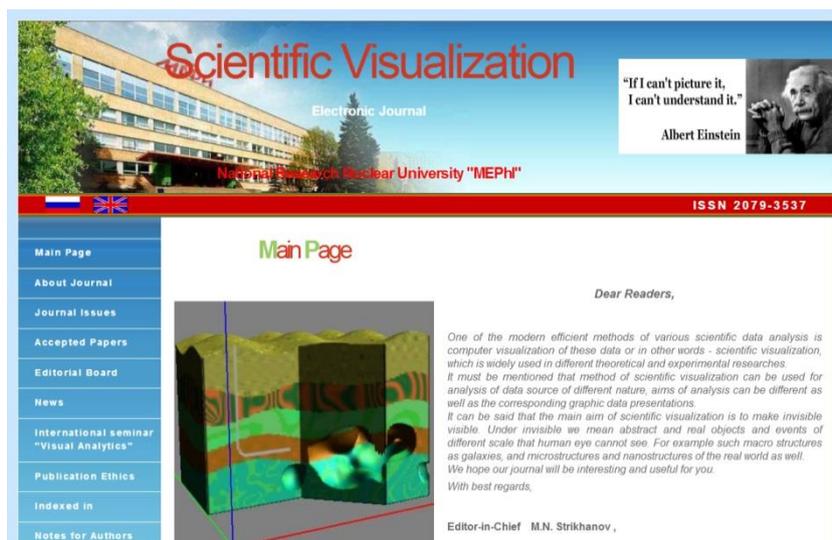


Figure 8. Main page of the “Scientific Visualization” Internet-journal

The NRNU “MEPhI” (Moscow, Russia) has been publishing the “Scientific Visualization” Internet Journal (<http://sv-journal.com>) since 2009. Materials published in the Journal are devoted to different aspects of computer scientific visualization development and application of its tools and methods. Materials are published as papers and short communications. Authors may use English or Russian as publication language. The title of an article, the list of authors and the abstract are presented in both English and Russian languages. The primary aim of the Journal is to publish high quality original works on computer scientific visualization. Previously published works are not acceptable unless there is considerable update.

The editorial board consists of visualization specialists from Russia, USA, UK, Japan, France, Singapore, Netherlands and Switzerland. The journal is indexed in Scopus, Compendex and Russian Science Citation Index. We have to note that university researchers including PhD and master degree students actively publish papers in the journal. Also, the journal is recommended as an educational source for s PhD students of the mentioned “The Scientific Visualization” course.

5. Conclusion

As conclusion, we would like to say that scientific visualization attracts a lot of attention in the NRNU "MEPhI", one of the leading Russian universities.

The works in this field are carried out in three related directions: Scientific Visualization in Physics Research, Scientific Visualization in Physics Education and “Scientific Visualization” Journal Publication.

These works are followed by research of theoretical aspects of modern Scientific Visualization for scientific data analysis. All these activities are carried out in international collaboration with involvement of leading Russian and foreign specialists.

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