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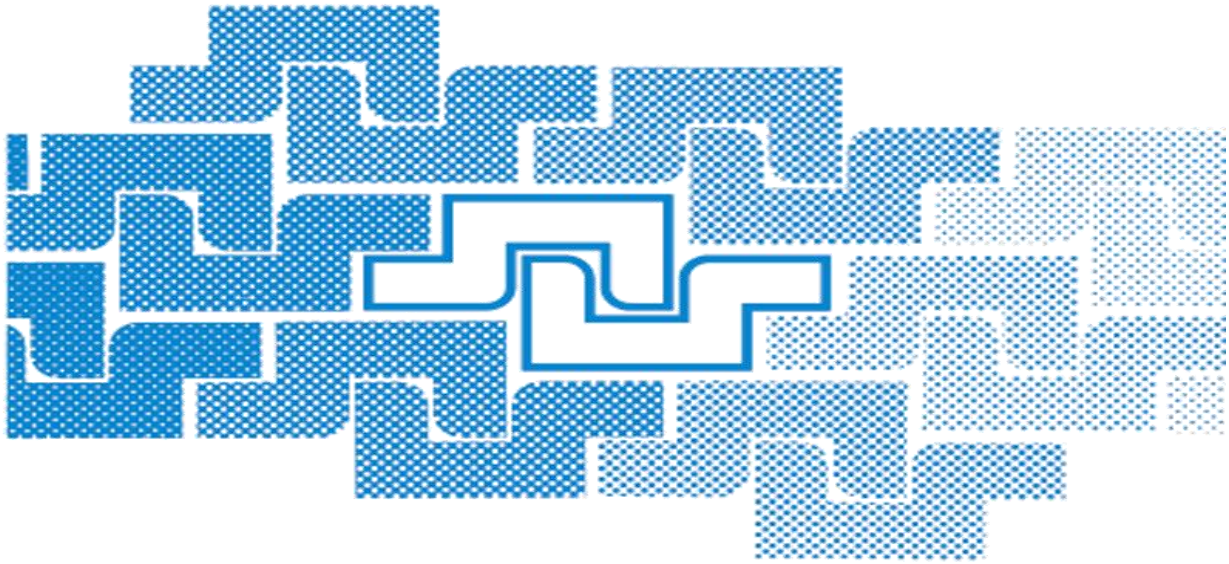

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This monograph highlights new approaches to the development of modeling and complex processes in nanostructures and nanoporous media based on high-performance parallel computing, supercomputer technologies of computational mathematics tools. The design of the systems under consideration is based on new science-intensive technologies of object description, new computational solutions taking into account the architecture of computer systems and software.

For scientists, specialists in the field of applied mathematics, mathematical modeling, high-performance parallel computing and software engineering, teachers of higher educational institutions, postgraduate students, engineers and students.

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INTRODUCTION

The development of nanophysics in recent decades has led not only to new fundamental knowledge of an academic nature, but also to the creation of new nanotechnologies with unique precision characteristics of such nanodevices as quantum cascade lasers and detectors. In connection with the exceptional capabilities of nanodevices in physics, chemistry, engineering, biology, medicine and other sciences, the very word "nano" has gone far beyond the lexicon of professional physicists. It became frequently used not only by scientists of various fields, but also by politicians.

One of the fields of nanotechnology that continues to develop intensively is the creation of such quantum cascade lasers (QCL) and quantum cascade detectors (QCD) that operate in the current terahertz frequency range of electromagnetic waves. Since the elemental basis of these nanodevices are multilayered open resonant tunnel structures (RTS), the study of the transport properties of electron flows through these structures is an extremely urgent task. After all, only a sufficiently developed theory of physical processes that occur when charged quasi-particles pass through RTS with electric, magnetic and electromagnetic fields can be a reliable basis for the conscious choice of such a geometric design of cascades, which will allow optimizing the operation of KKL and KD.

The last chapter of the boock highlights development of methods and algorithms for studying mathematical models with approximate data of sparse structure on the latest high-performance computers with parallel organization of calculations of different architecture. A new methodology for studying mathematical models with approximate data of sparse structure on the latest high-performance parallel and distributed computer systems using multilevel parallelism is developed. An approach is proposed to solving nonlinear problems on supercomputers, which arise in the mathematical modeling of the strength and stability of structures, in particular in the modeling of the life cycle of responsible welded structures of energy objects. Block and block-cyclic algorithms for parallel computations for solving linear algebra

problems with sparse matrices on the basis of structural regularization and decomposition of sparse structure data is developed and investigated. Problems of linear algebra (systems of linear equations and matrix problems on eigenvalues) are a significant part of mathematical modeling. Improving the quality of mathematical modeling is directly related to increasing the productivity and efficiency of modern parallel computing systems. The key point in solving these problems is the choice, development and application of methods for automating the design of parallel programs for mathematical modeling, as well as software tools for configuring the developed programs on various high-performance computing platforms, which include multi-core and cluster architectures - graphics processors, "cloud platforms", etc.

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