Development of Multiscale Hierarchical Simulation Package MULTICOMP

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Nanotechnology is an emerging field of science and technology dealing with the control of matter at the atomic and molecular levels. Therefore, like in any innovations, its development requires the theoretical elaboration of ideas, methods and models. This is impossible without computer simulation and design. Since nanotechnology deals with the creation of new materials with a given atomic and molecular structures by controlled manipulation of atoms and molecules, the use of methods of multiscale modeling is principally required. On the other hand, many processes in materials and product characteristics are more convenient and easier to describe at the macro level, without going into details of the atomic and molecular structures of the substance in question. This supposes the use of phenomenological models and macroscopic characteristics of the medium. Such features of nanotechnology lead to understanding of its multiscale and multiparametric background, which should be reflected in the corresponding methods of computer simulation. In this regard, it became important to develop methods for computer design, covering various levels of the description of nanomaterials — from atomic-molecular level to meso- and macroscopic levels. This will allow one to intentionally create new materials and products with desired characteristics by the manipulation of single atoms, molecules, and nanoparticles.

The report discusses the development of the Multiscale Hierarchical Simulation Package MULTICOMP, which contains a set of physicochemical and information models and programs. MULTICOMP makes it possible to design nanostructured materials on different scales: (1) atomic and molecular, (2) supramolecular, (3) nano, and (4) micro scales.

The main approach used in MULTICOMP is based on the fact that nanomaterials have a hierarchical structure, i.e., the structure of the lower level is built into the structure of a higher level. The direct simulations for complete time and space scales (which are impossible with current computer resources) are replaced by simulations on each scale level with the end-to-end transfer of the calculation results (structure and properties) from the lower level of the structure scale to a higher level. The major advantage of MULTICOMP is ability to generate different kinds of nanomaterials and to simulate them starting from chemical formulas and recipe of material. At each next level, the results of the previous level are used as input parameters, and the simulation uses physical models and methods specifically designed for the corresponding space and time scales. All parameters are automatically transferred between simulation levels, which is also an important feature of MULTICOM because it is not implemented in other packages and usually require direct user involvement. In the future, we intend to realize in MULTICOMP to transfer data not only from below up, but from top to bottom as well.

The simulation process in MULTICOMP is carried out in a quite simple and intelligent way. A graphical user interface (GUI, see Figure 1) makes it easy to implement the simulations

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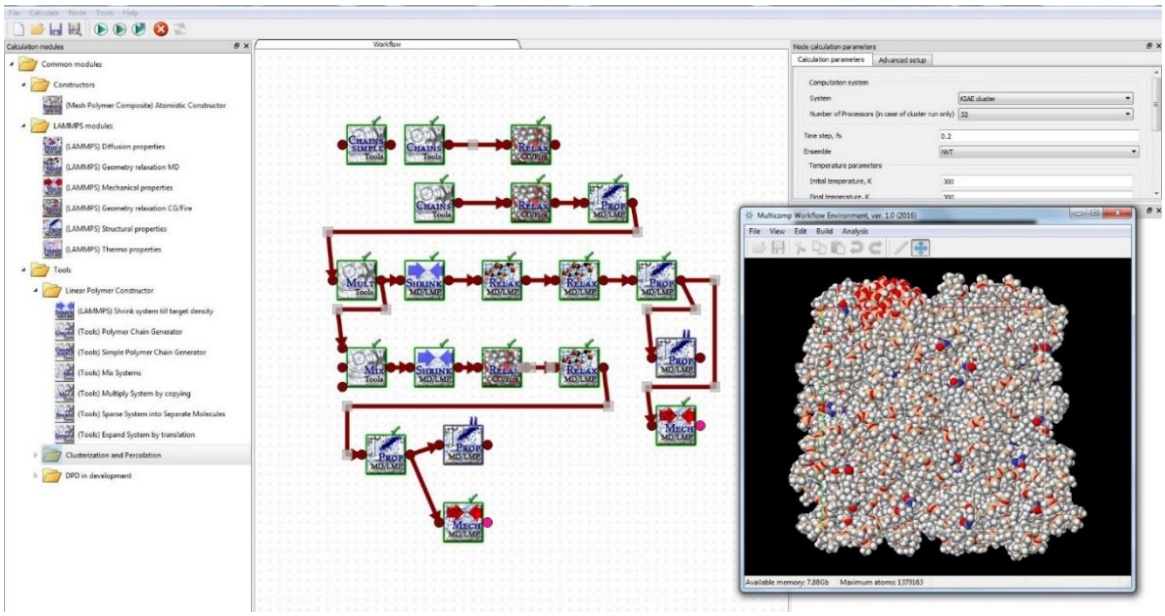

Fig. 1. The figure shows an example of a user's project for constructing a sample material of a polymer matrix with a nanoparticle created in the graphical user interface of MULTICOMP. The user can specify the sequence of starting the computational modules (represented as tiles), determine the data transfer between the modules (the arrows connecting the tiles), select the number of processors and execute them all together or separately. Each module allows calling up graphical and text editors to enter and change module parameters, control the progress of calculations, import/export calculation results, view calculation results and log files.

from the building blocks (monomers, polymer chains, nanoparticles, surfaces, etc.). The information exchange between the modeling levels is carried out using parsers, which automatically extract the required data from the output files (which contains information about resulting chemical structures) of the developed program modules or external programs and transfer the data to other program modules (or external programs) for further processing.

All simulation strategies and models as part of MULTICOMP are adapted to high performance parallel computing environments and can operate on currently available multi-teraflop/petaflop computational resources. The performance of the simulations is determined by remote computer facilities on which the server part of the MULTICOMOM is installed and the resources available to users (number of nodes, number of jobs etc.). It can communicate with SLURM and PBS submission systems. Parallel implementation of simulation modules depending on their purpose are based on data (small molecular systems) or domain (large molecular systems) decomposition techniques.

People from different areas such as academic researchers and industrial developers can use MULTICOMP. It provides technical ability to simulate the filled polymer systems containing up to several millions of atoms using fully atomistic molecular dynamics, to simulate coarse-grained nanocomposite models on length scales up to 10 μm and on time scales up to 100 μs. As a result, researches can simulate, verify and analyze the performance of different polymer nanocomposites to evaluate the effect of different parameters on material properties, thereby improving processing recipes. In its turn, this will provide deeper insights into the complexities and the mechanics necessary to build full-scale virtual prototyping systems covering the whole design process, thus allowing engineers to get a better understanding of what is needed in the industry.

The performance of the package is currently being tested on the Kurchatov Institute cluster. As an example of using MULTICOMP, we also present in our report recent results on simulation of the different polymer matrixes and nanocomposites.