Russian Supercomputing Days

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# MultiComp: Software Package for Multiscale Simulations

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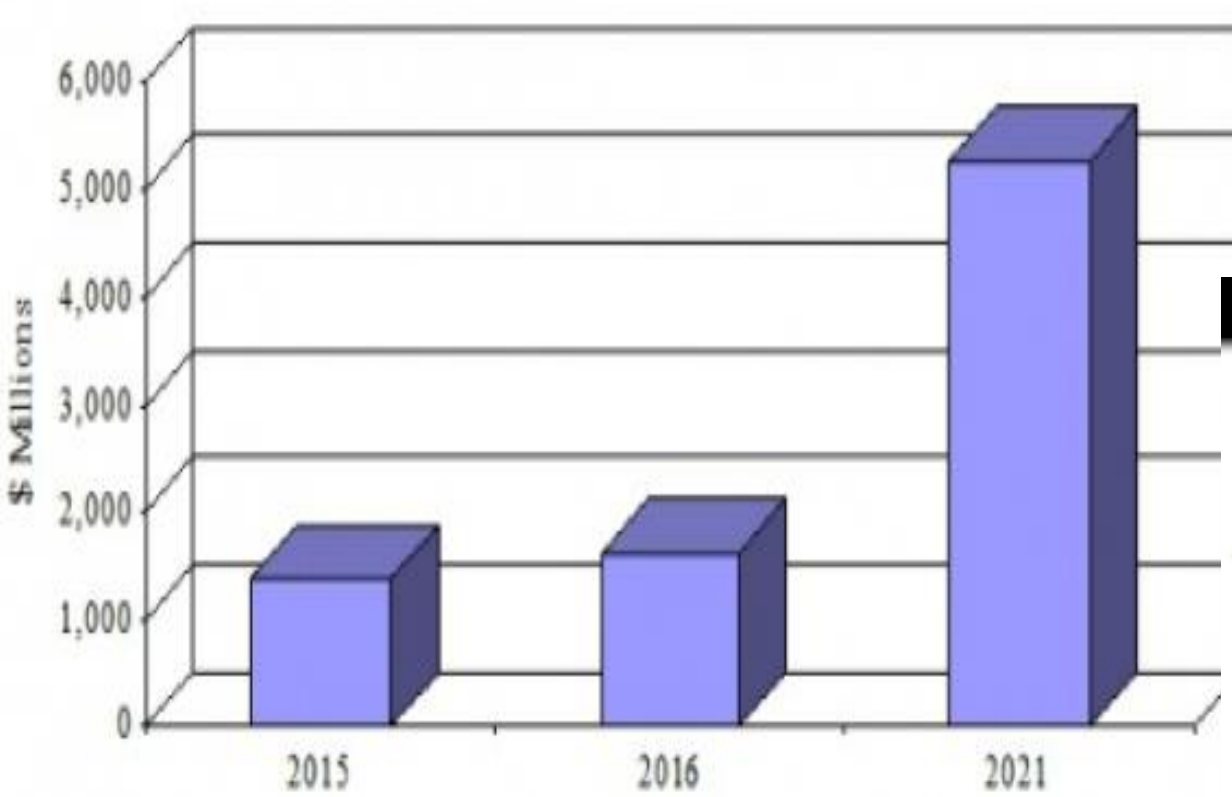
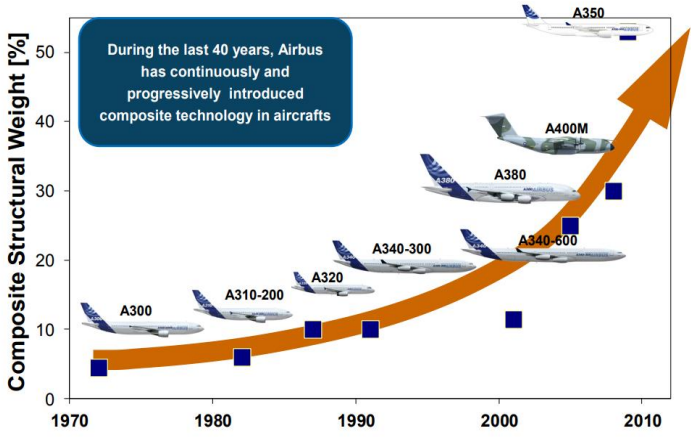
The work is performed on the basis of Kintech Lab Ltd.

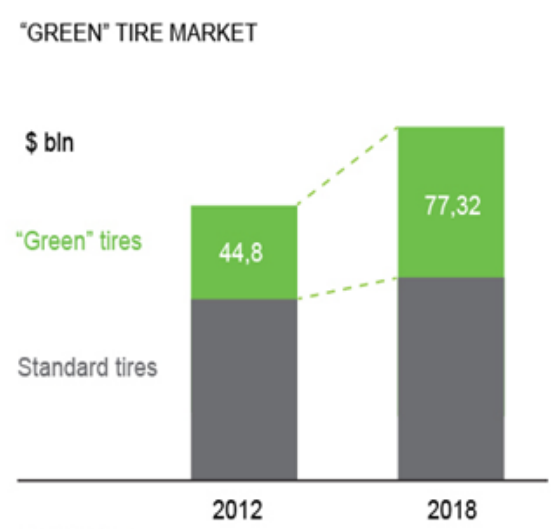
# the need for the design of new nanocomposites

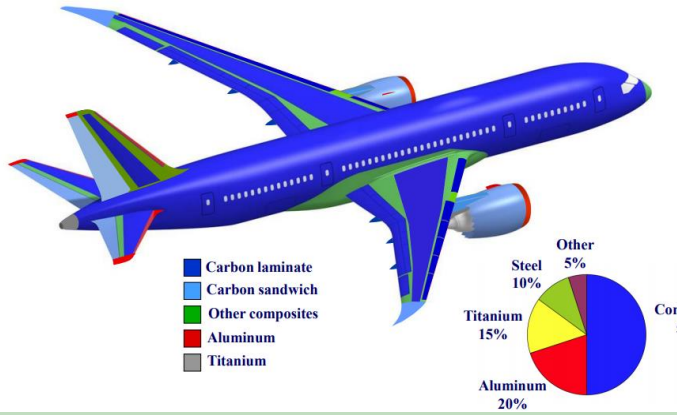
**The volume of the world market for nanocomposites in 2015-2022, $ million**

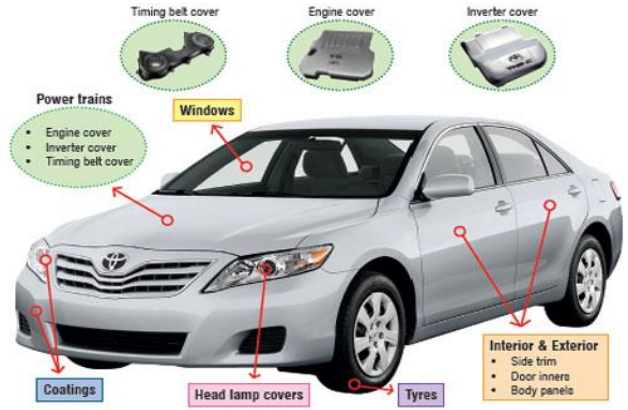




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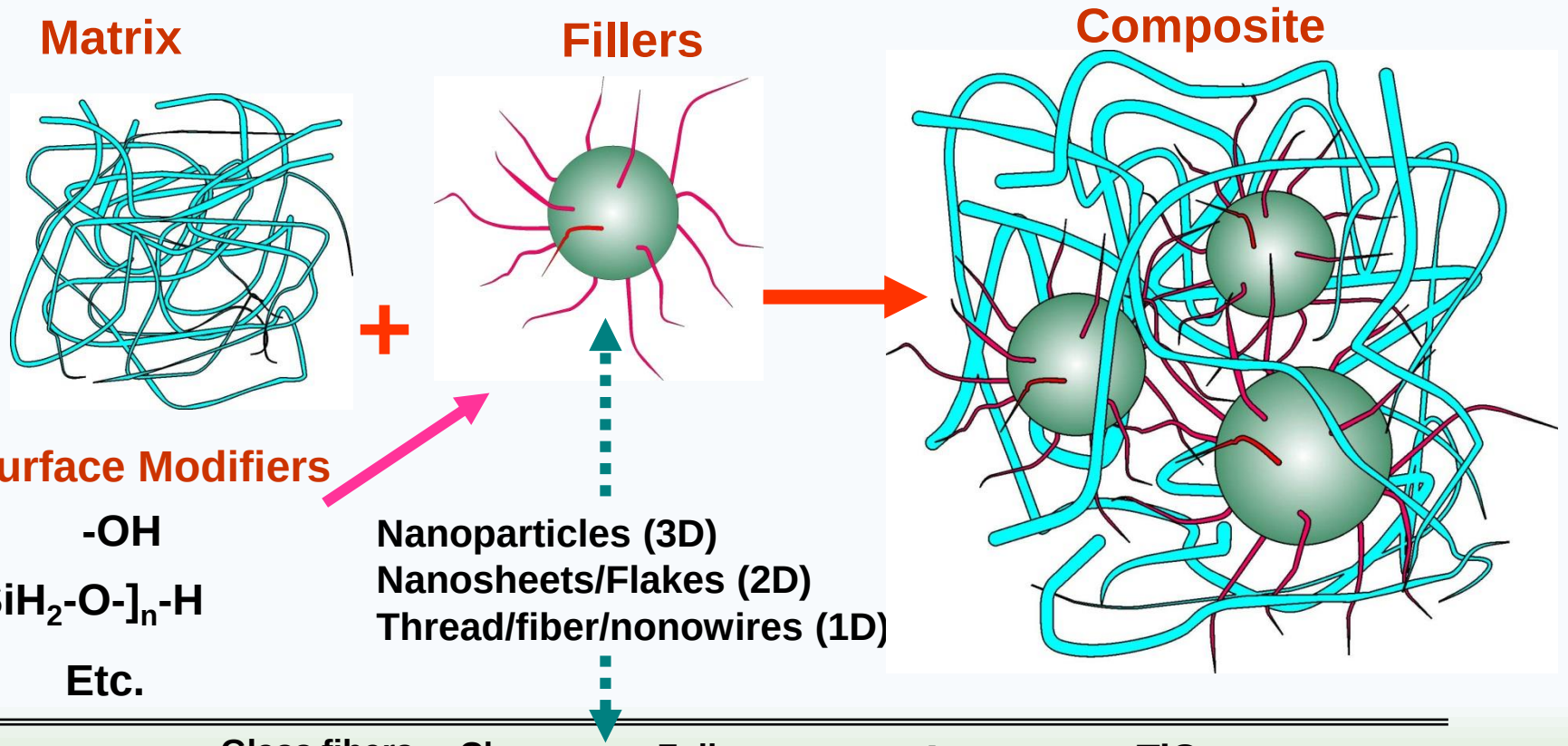
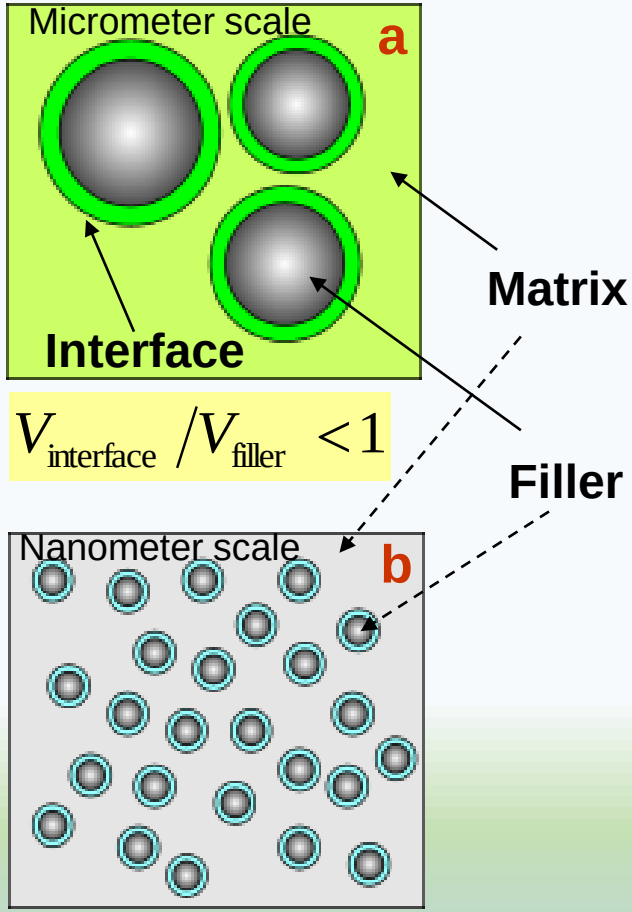
# what is polymer nanocomposites?

Combination of a polymer matrix and filler that have at least one dimension (i.e. length, width, or thickness) in the nanometer size range (1 nm = $10^{-9}$ m)

- **Composites** are materials consisting of two or more physically different phases, the combination of which leads to the emergence of new unique properties that differ from the characteristics of the original components.

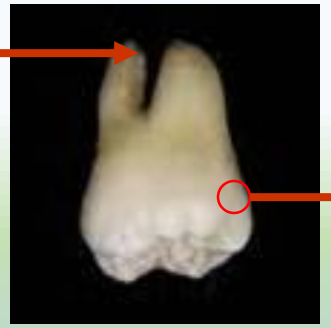


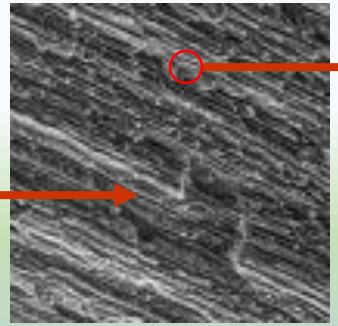




# why polymer nanocomposites?

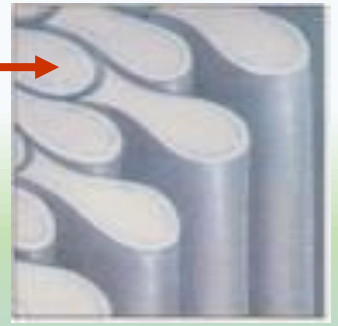
- Possible to achieve combinations of properties not attainable with metals, ceramics, or polymers alone
- The key problem of polymers is low elastic modulus (polymers ~2GPa, glasses ~80, metals ~100GPa) , low termostability and etc.
- The nanoparticle provide reinforcement of polymer matrix
  - Example: **tooth enamel** (largely calcium phosphate) has the **elastic modulus 83GPa**

Tooth enamel is an instance of natural polymer nanocomposites





model of the enamel

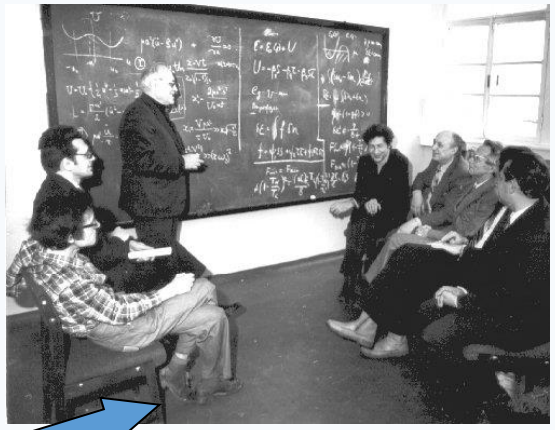


Tooth enamel at 1000X

# computer simulations in new materials design

Experimental Study

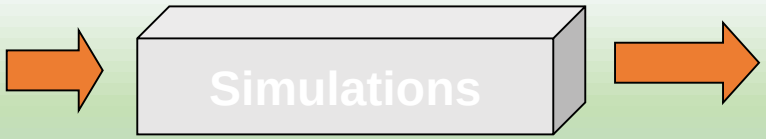
Computer Modelling



Theory

What can we do with using computer modelling?

**Input**
Chemical structure, Quantitative ratios, Physical environment




**Output**
**Structure**
**Young's modulus**
**Tg, Thermal conductivity**
**Ets …**

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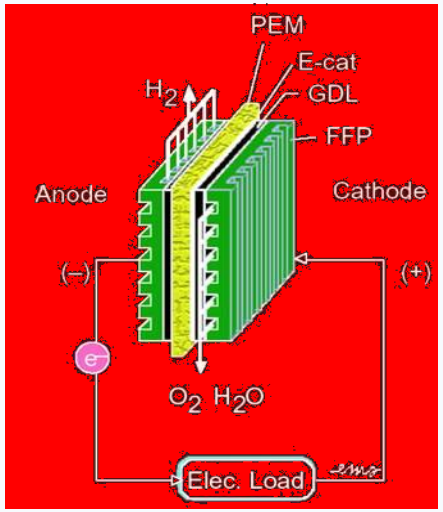
# multiscale nature of polymer




**technological level**

Characteristic Times

complete process

years

hours

minutes

seconds

micro seconds

nano seconds

pico seconds

femto seconds

engineering design

continuum

finite element method

continuum

Mesoscale

coarse-grained models

MC MD

molecular ensembles

QM

molecules

1 A

1 nm

1 mm

1 mm

m

Characteristic Scales

In the case of nanocomposites, it is impossible within the framework of a one-level approach to combine high accuracy and large scale of consideration.

- **Atomistic level** - properties of nanosized filler and phase interaction
- **Mesoscal**e - the distribution of the filler in the matrix
- **Macro level** - effective material properties

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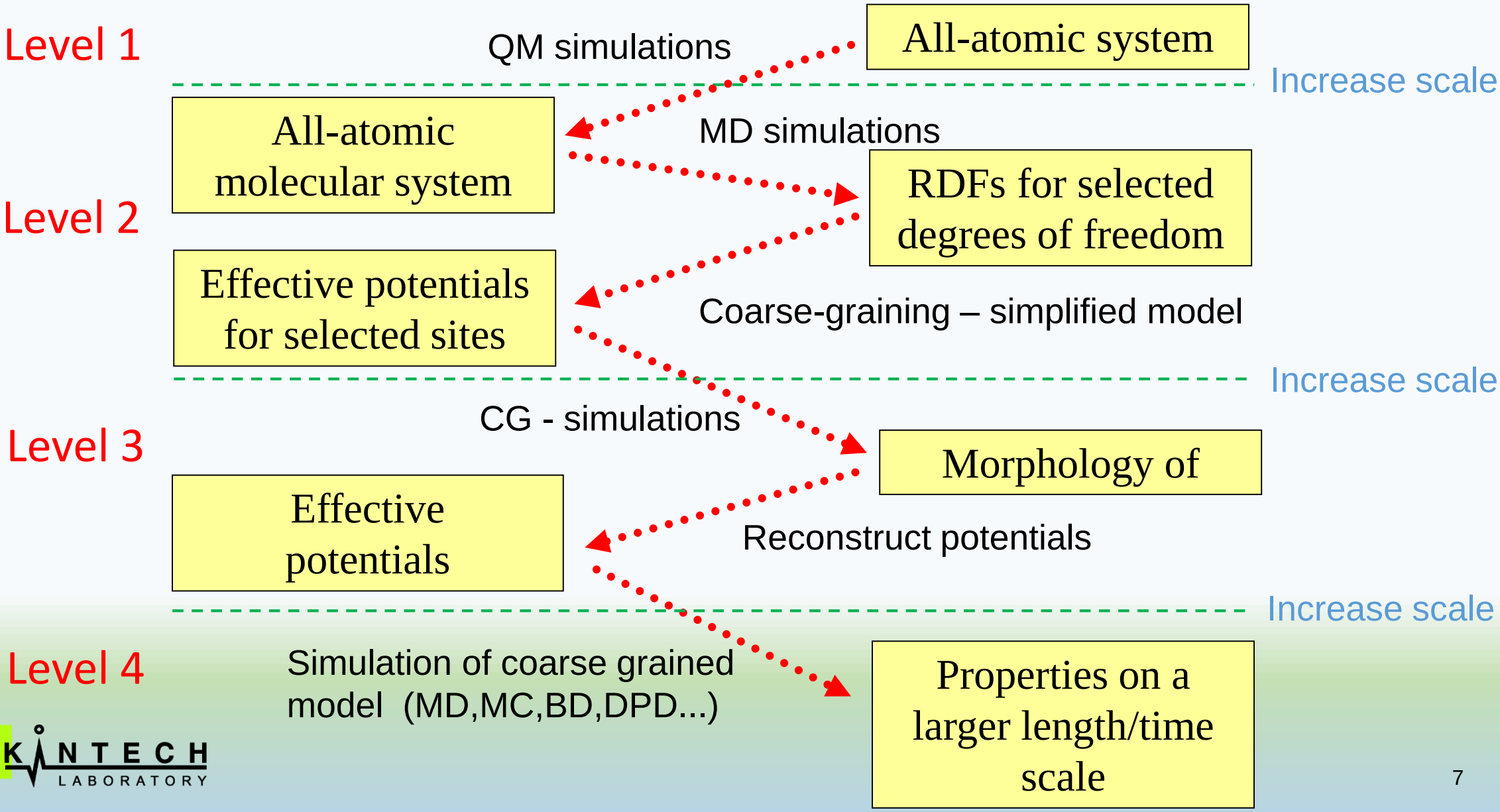
# multi-scale modeling approach



# software packages & nanocomposites

## freeware

- **PACKMOL**
- **OCTA Project**
- **CASTEP**
- **LAMMPS**
- **SCD Materials Modeling Software** DL_POLY, DL_MESO
- **Computational Soft Materials (COMSOFT) Workbench**

## commercial

- **Materials Studio (BIOVIA) DIGIMAT (MC Software)**
- **Materials Science Suite (Schrodinger LLC)**
- **GeoDict (Math2Market Gmbh)**
- **COMSOL Multiphysics (COMSOL)**
- **MAPS (Material and Process Simulation) (Scienomics)**
- **ADF Modeling Suite (Software for Chemistry & Materials B.V. (SCM))**
- **Mode A Software (Materials Design Inc.)**

The software package should have flexible capabilities for relatively fast construction of various variants of nanomaterial samples, depending on the input parameters.

# Multicomp software package for multiscale modeling of the properties of polymer nanocomposites

## Purpose

- Used for multilevel predictive modeling of morphology, thermal and mechanical properties of nanocomposites with a polymer matrix
- The package is specially designed for high-throughput screening of materials based on supercomputers
- Allows you to predict various material properties:
  - structural
  - mechanical
  - thermophysical
  - transport

## Advantages

1. Effective scientific workflow for computing automation
2. Integration of models for calculating the properties of nanocomposites with micro-, meso- and macrolevels
3. Client-server architecture for leveraging remote high performance computing (HPC) resources
4. Open architecture: compute modules can be added, modified and replaced without developer assistance
5. Flexibility in adaptation and configuration
6. Convenient graphical user interface
7. Visual 1D-2D-3D-visualization of calculations

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# multilevel modeling in the scientific workflow concept

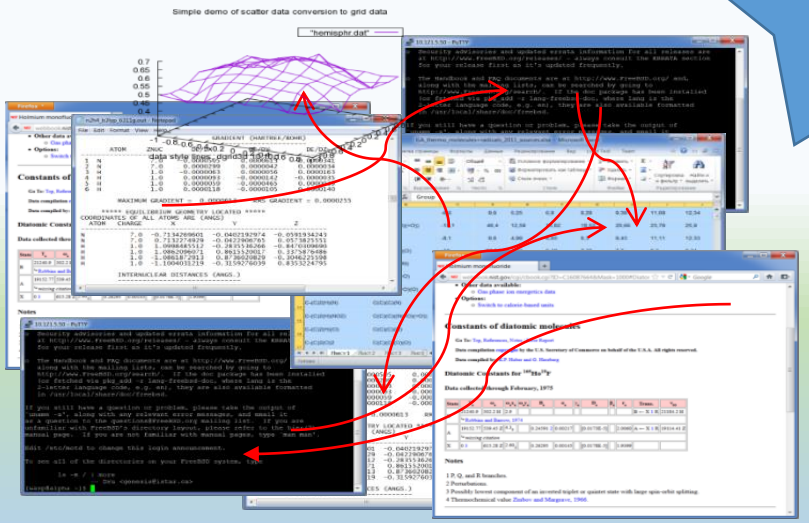
## Problems with old approaches

A large number of programs
- Atomistics (Lammps, Gromacs, DLPoly)
  Mesoscale (DPD)
- Macro Level (FEM)

Various means of processing results
- Excel
- Gnuplot, Matplotlib
- Jmol, Ovito

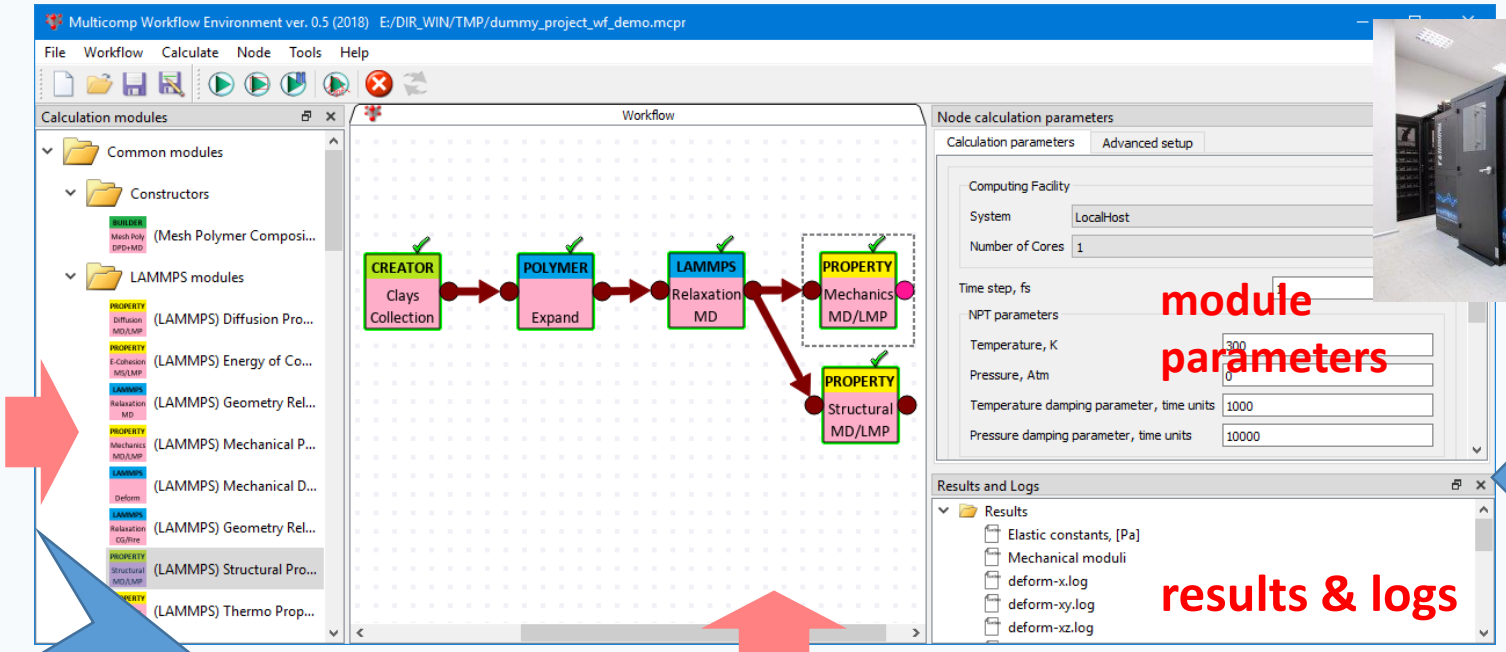
Incompatible formats

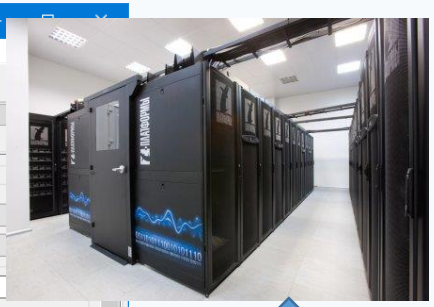
Script Sets




**modules kit**

Supercomputer



**module parameters**

**results & logs**

**Internet**

**Calculation scenario constructor**

## Benefits of the Scientific Workflow Concept

- Open architecture: the user can add, modify and replace computational modules without developer assistance
- Multi-user collaboration and data exchange
- Data exchange between modules based on templates
- Highly scalable performance
- Flexibility in adaptation and configuration
- Isolating Modules: reduces risk and reduces impact on the whole system

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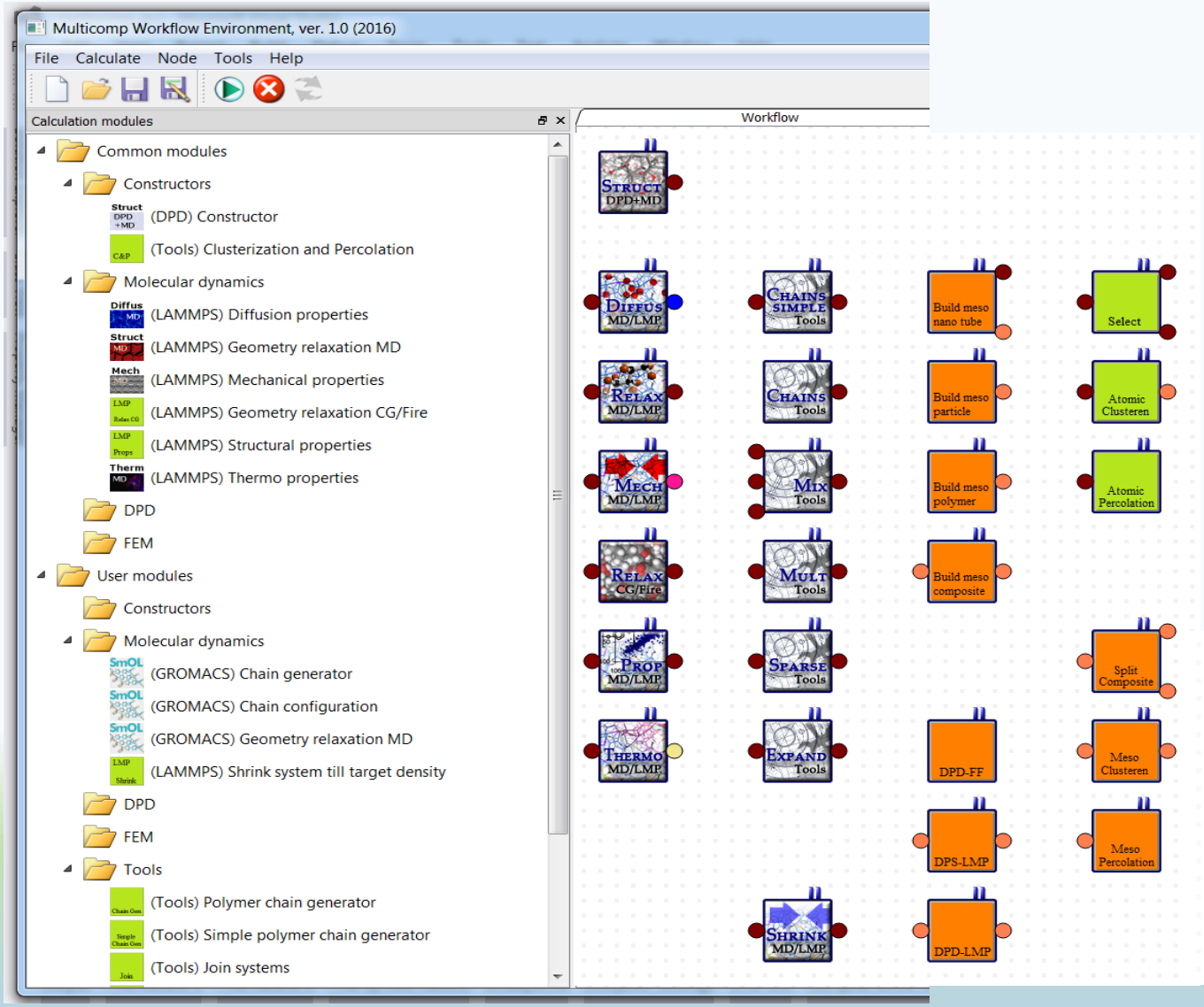
НАУКА И ИННОВАЦИИ

# modules kit




## constructors

Nano/Meso tube Generator

Atomistic Constructor (K23)

Linear Meso-polymer Generator and Mixer

## service tools

Simple Polymer Chain Generator

Polymer Chain Generator

Multiply System by copying

Expand System by translation

Join Systems.

Sparse System into Separate Molecules

Mix Systems

Select and Split

## simulations tools

Geometry relaxation CG/Fire

Geometry relaxation MD

Shrink system till target density

Meso Structure Relaxation MD

Meso Structure Relaxation CG

## calculation and analysis of properties

Mechanical properties

Thermo properties

Diffusion properties

Structural properties

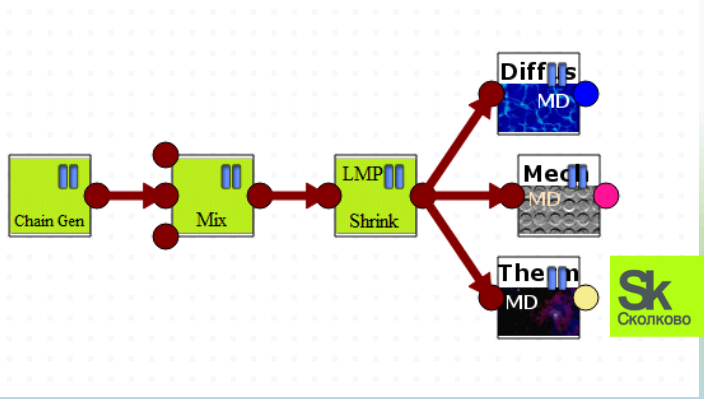
(density, RDF, XRD, SAED, porosity)

Clusterization

Percolation

Atomic Percolation

Mesoscopic Percolation

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# data storage format

- Based on the analysis of the development and application of existing multiscale modeling packages, the developers of the package concluded that the XML format is the most convenient way of storing and exchanging data in the process of multilevel modeling.
- The data within the complex is stored in a structured form and saved in XML format.
- The graphical user interface of the complex allows you to view and edit these data, as well as add new ones.
- In addition, through the interface, it is possible to import data into the complex from the output files of external programs.

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</species_molecule_name01>
```

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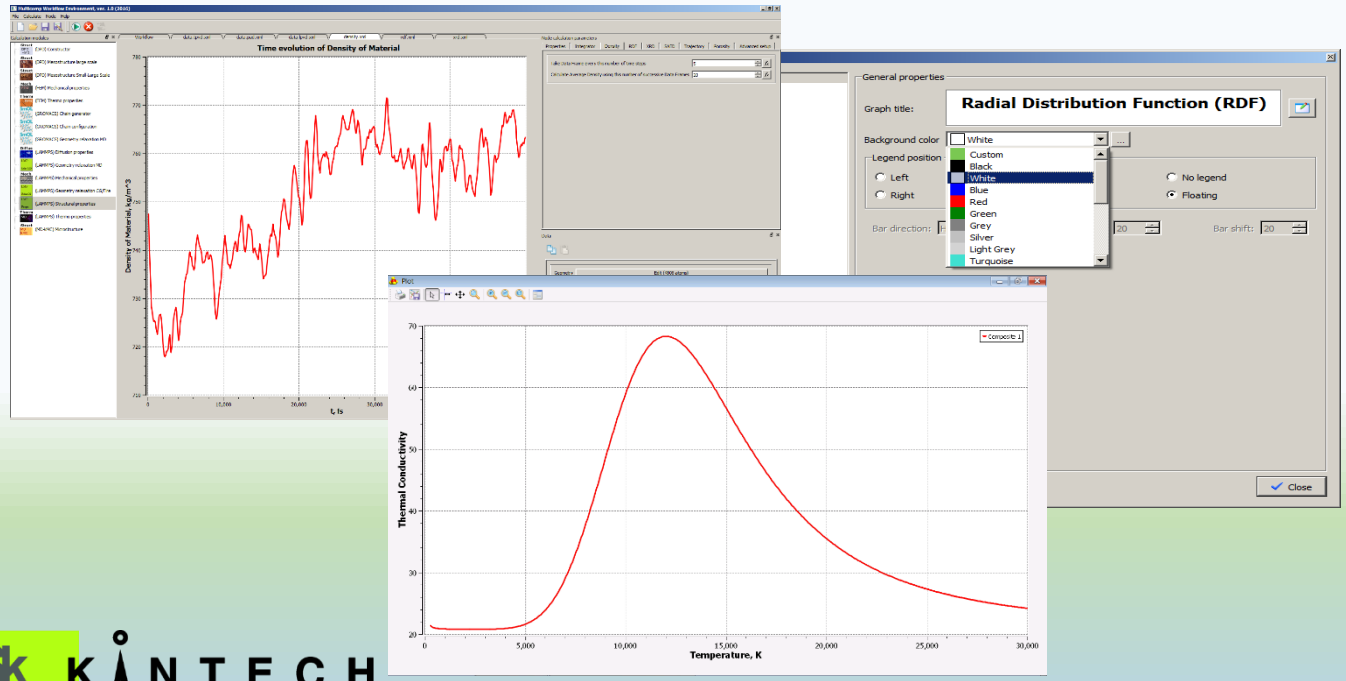
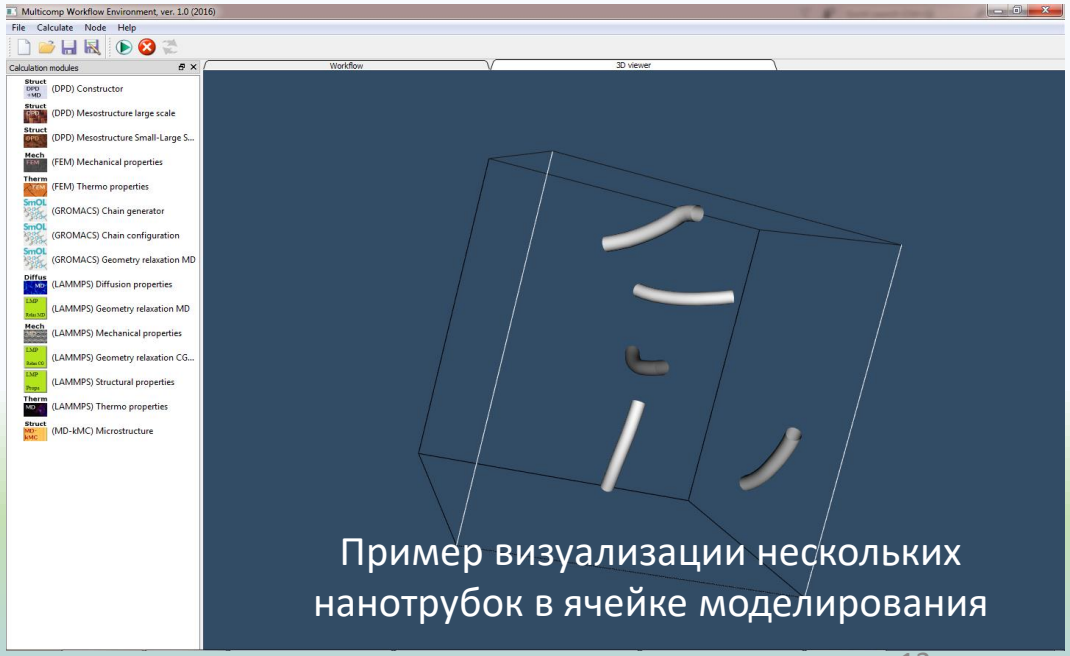
# visualization

- The results are displayed using an interactive 1D / 2D / 3D visualization module consisting of 2 blocks: 1D visualization and 2D / 3D visualization.
- Block 1D visualization consists of an embedded window for displaying functional dependencies, a separate form containing a display window and a toolbar, a window for setting display parameters and auxiliary windows.
- The 2D / 3D visualization block consists of a built-in window for displaying 2D / 3D objects and grids and a separate form containing the display window, the main menu and the toolbar.

**embeddable window for displaying functional dependencies**

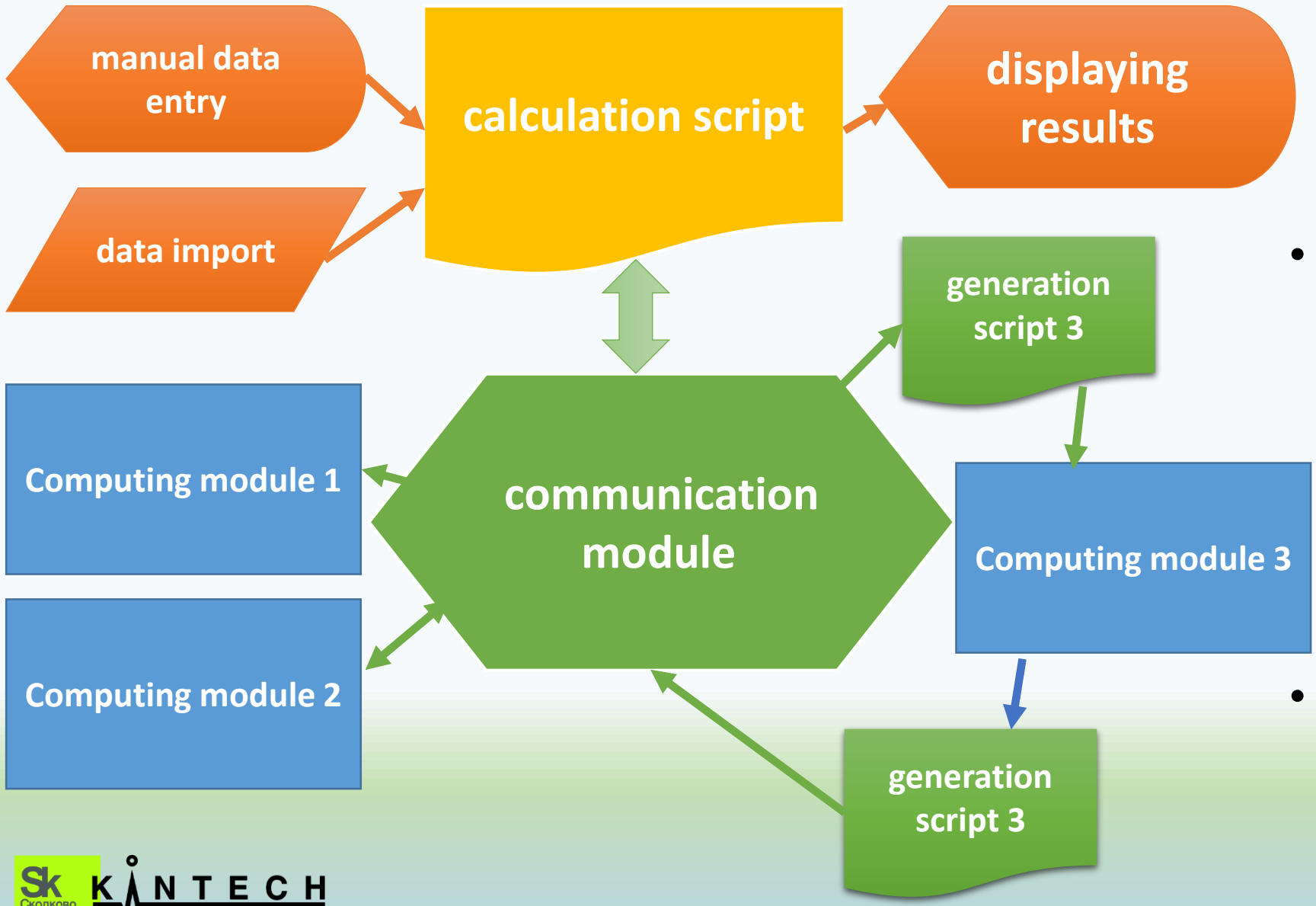



**embedded 2D / 3D object and mesh display window**




Пример визуализации нескольких нанотрубок в ячейке моделирования

# data exchange




- Calculation modules can directly support the XML format of the batch calculation script file as the format of their input and output files.
- For computational modules that do not support the XML format, the input / output data are converted from the package format to the module format using the conversion control programs (scripts).
- The exchange module provides the corresponding API for the scripts to generate and read files.

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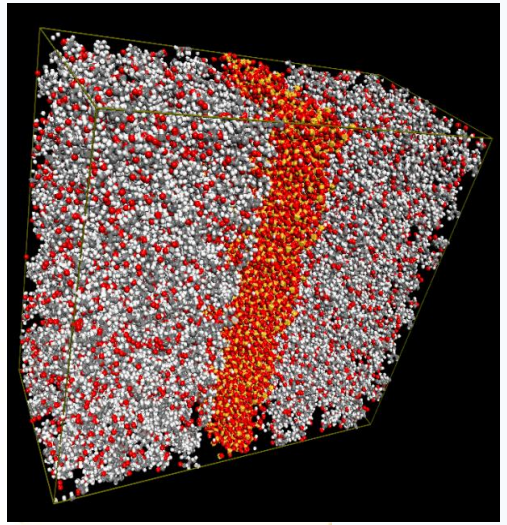
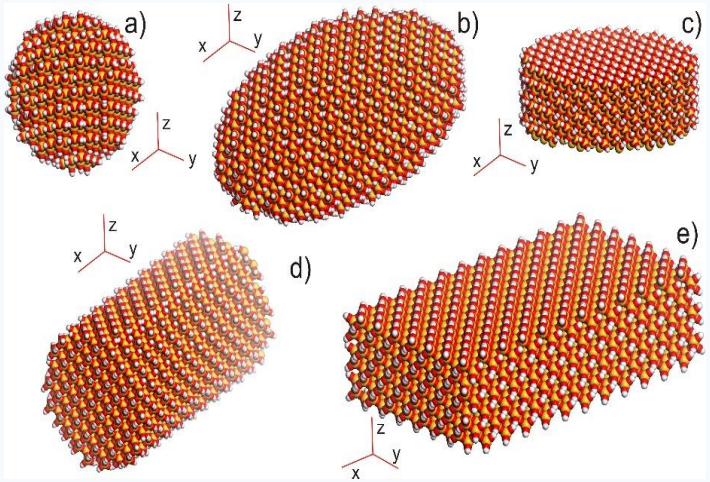
# constructor of epoxy based polymers and composites

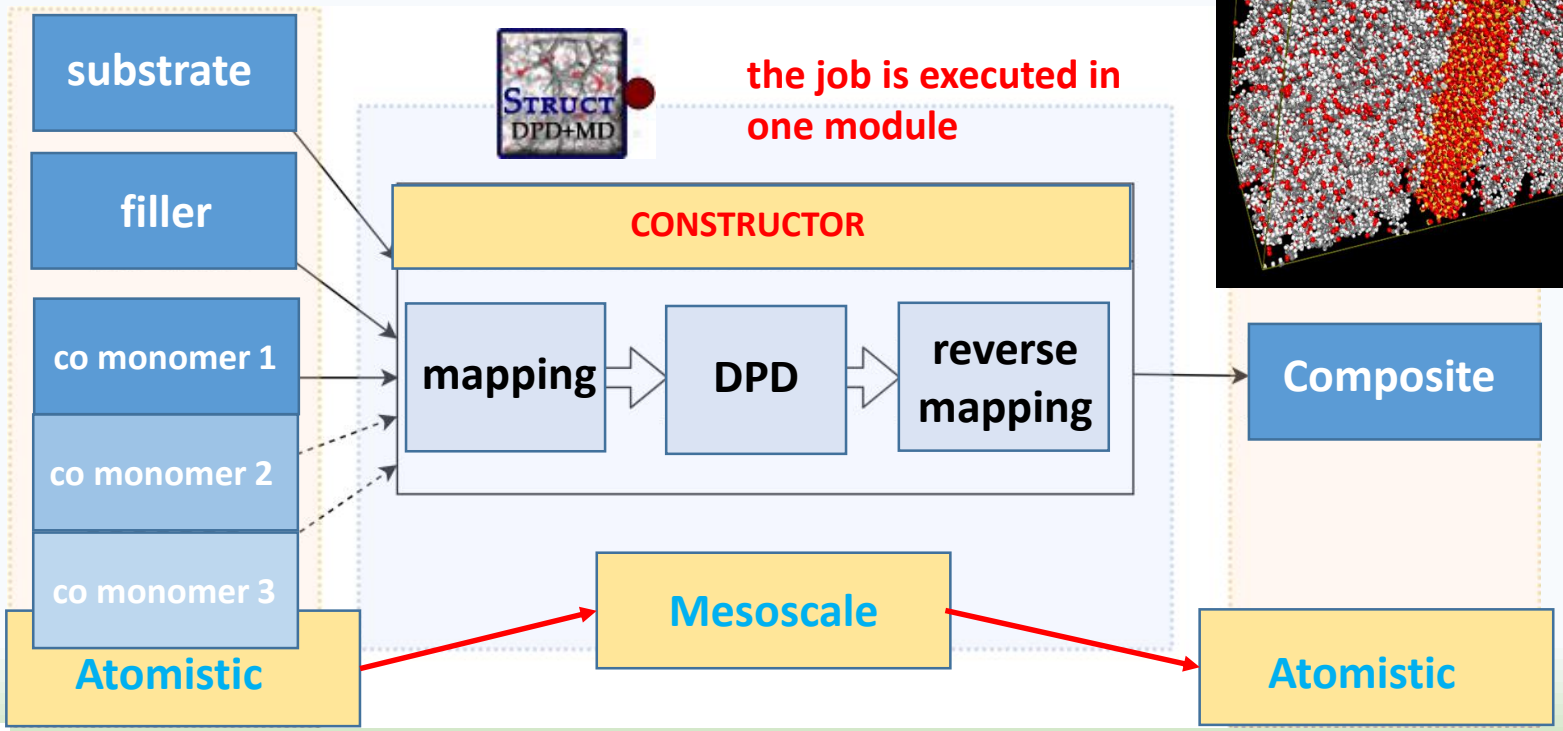
**Construction of epoxy based polymers and composites.**

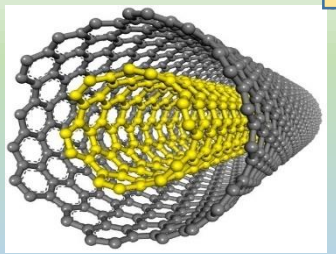
**Multilevel process running in one module:**

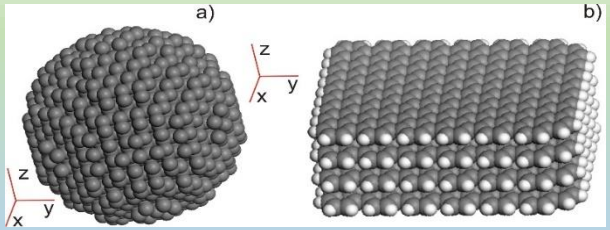
- Construction of an atomistic structure with the specification of filler particles, a substrate, and up to three components of a polymer matrix.
- Conversion of atomistic structure into structure for modeling by dissipative dynamics method at the mesoscale.
- Dissipative dynamics for the implementation of matrix crosslinking with preliminary and subsequent relaxation (Setting the cell size; controlling the reaction rates, the final degree of crosslinking).
- Reverse conversion of a structure to an atomistic one.

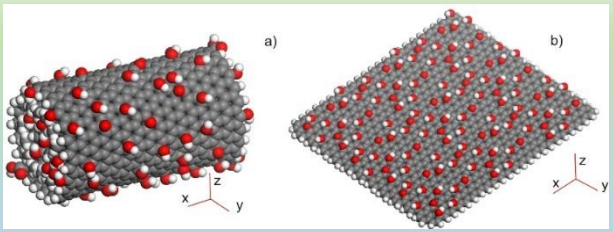




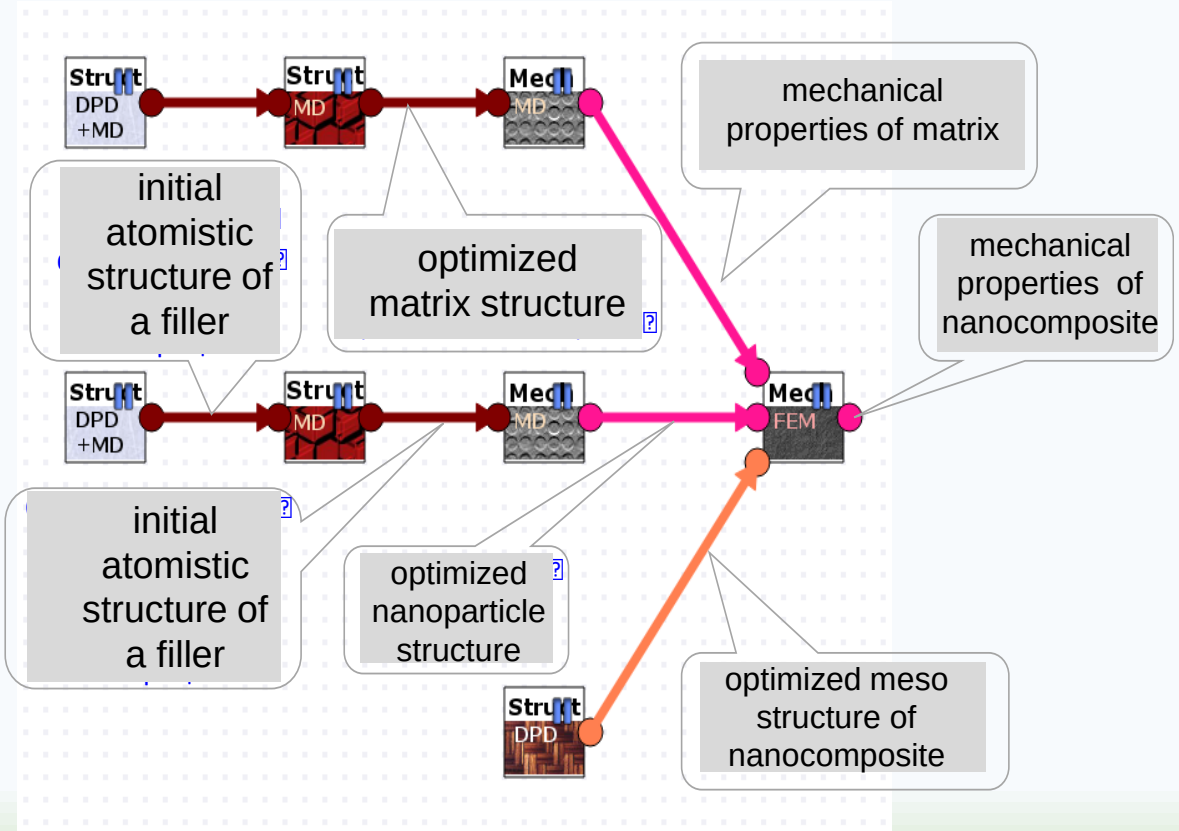





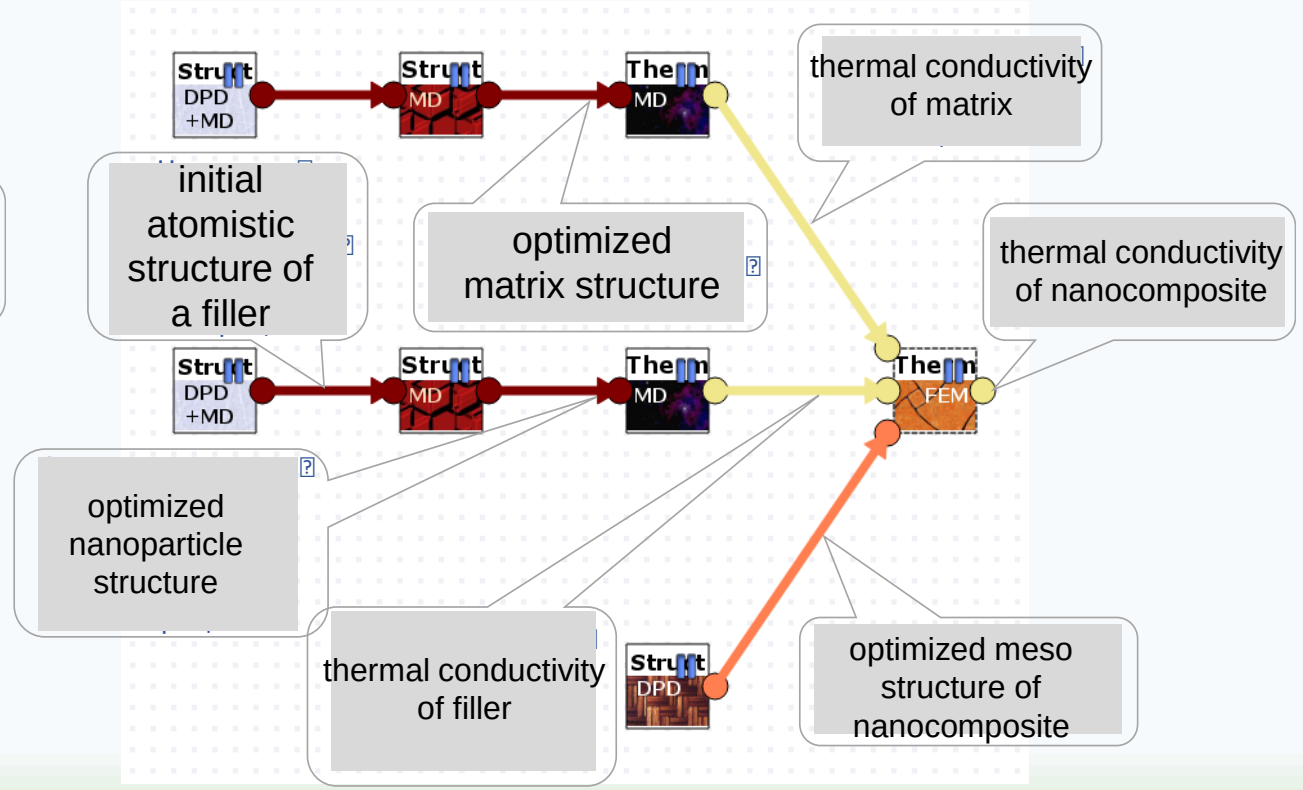



# scheme of data transfer between computing units

## mechanical properties




## thermal conductivity



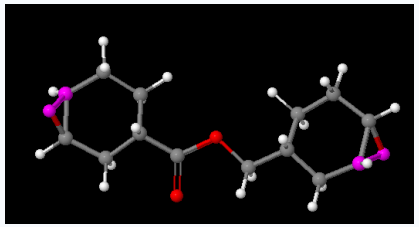

- Data transfer schemes provide the ability to carry out multilevel calculations of the physical properties of nanocomposites by transferring the calculation results between different levels of modeling. In this case, the data transfer formats developed at the previous stage are used.

# calculation of the mechanical properties of crosslinked epoxy matrices

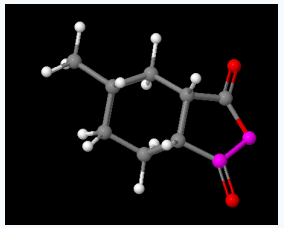
For crosslinked epoxy matrices, the literature shows a change in the modulus of elasticity depending on the degree of crosslinking [1].

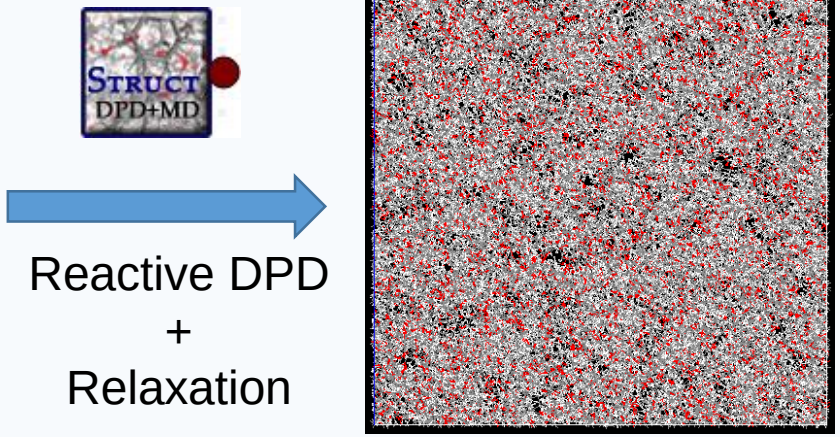
The morphology of polymer networks can be studied at the atomistic scale [2].

Epoxy monomer



Hardener







**Calculation script**

Using the constructor, it is convenient to study the dependence of physical properties on the degree of matrix crosslinking

| Conversion degree | Young's modulus GPa |
|---|---|
| 0.593 | 5.10 |
| 0.754 | 5.63 |

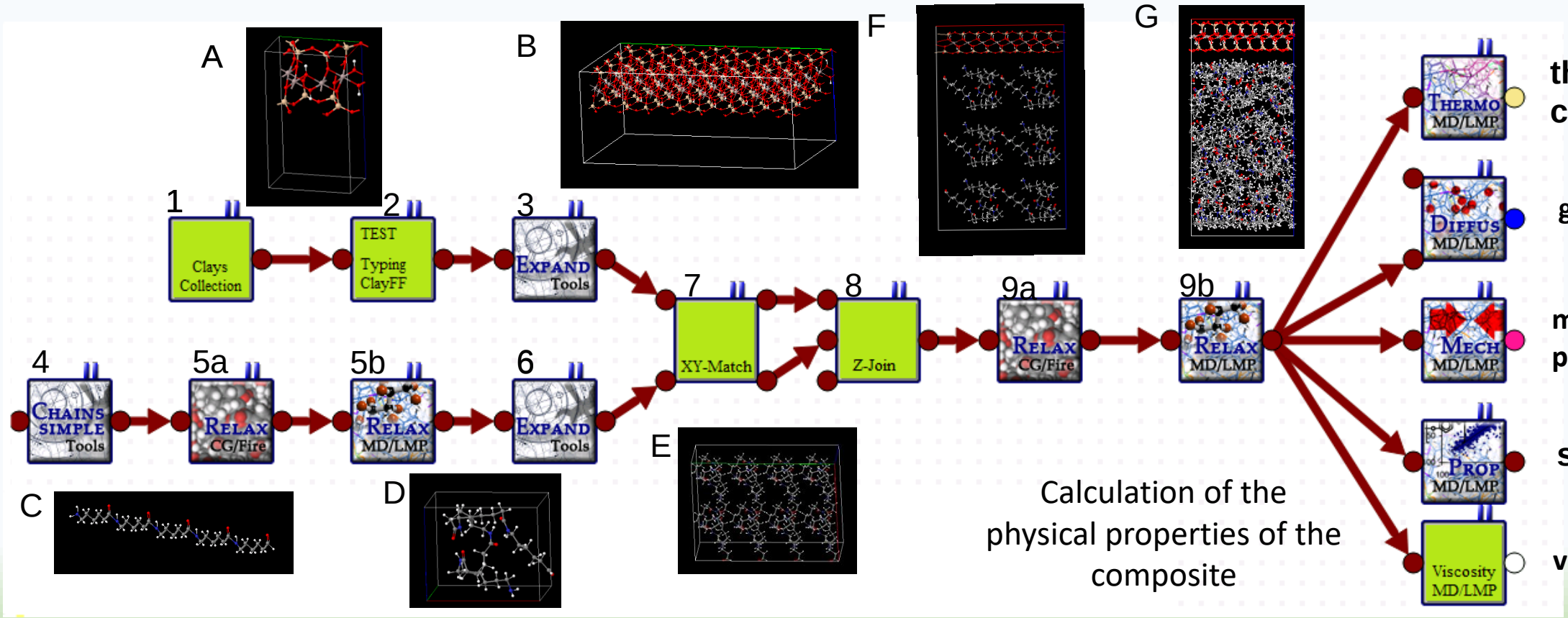

1 - Li C., Strachan A. Molecular dynamics predictions of thermal and mechanical properties of thermoset polymer EPON862/DETDA //Polymer. – 2011. – Т. 52. – №. 13. – С. 2920-2928.
2 - Komarov P. V. et al. Multiscale Simulations Approach: Crosslinked Polymer Matrices //Supercomputing Frontiers and Innovations. – 2018. – Т. 5. – №. 3. – С. 55-59.

# calculation of mechanical properties of organomodified montmorillonite intercalated with polyamide-6

**Generation of the atomistic structure of clay nanoparticles**

**Creation of a composite structure (connection of clay and polymer structures)**

filler 15%




**Generation of the atomistic structure of a polymer matrix**

**Elastic moduli obtained by calculation:**

EPA6 = 2.8 Gpa  EMMT = 232 Gpa  Ecomposite = 41 GPa

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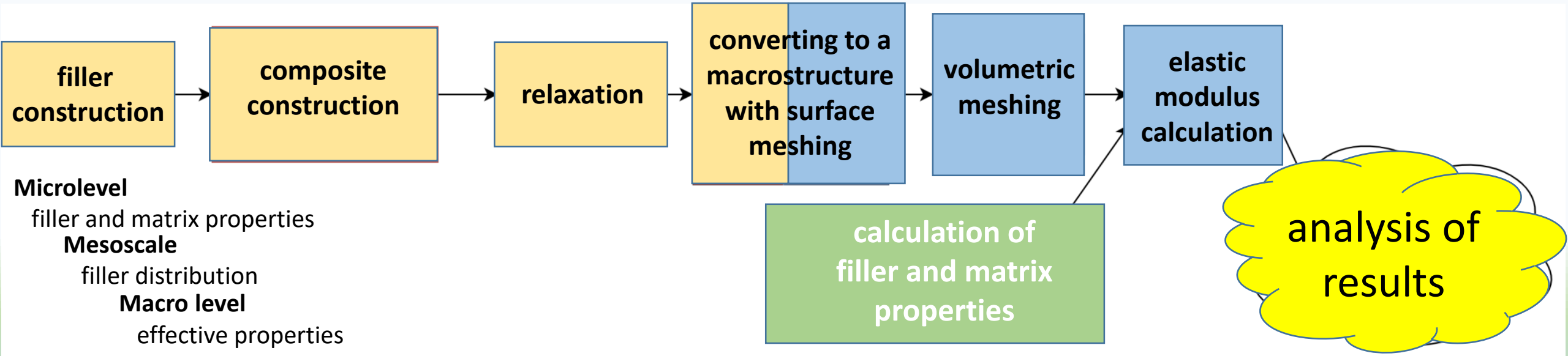
Skomorokhov A. S., Knizhnik A. A., Potapkin B. V. //The Journal of Physical Chemistry B. – 2019. – Т. 123. – №. 12. – С. 2710-2718.

# influence of the distribution of clay in the polymer matrix on the mechanical properties of the composite. simulation on three levels

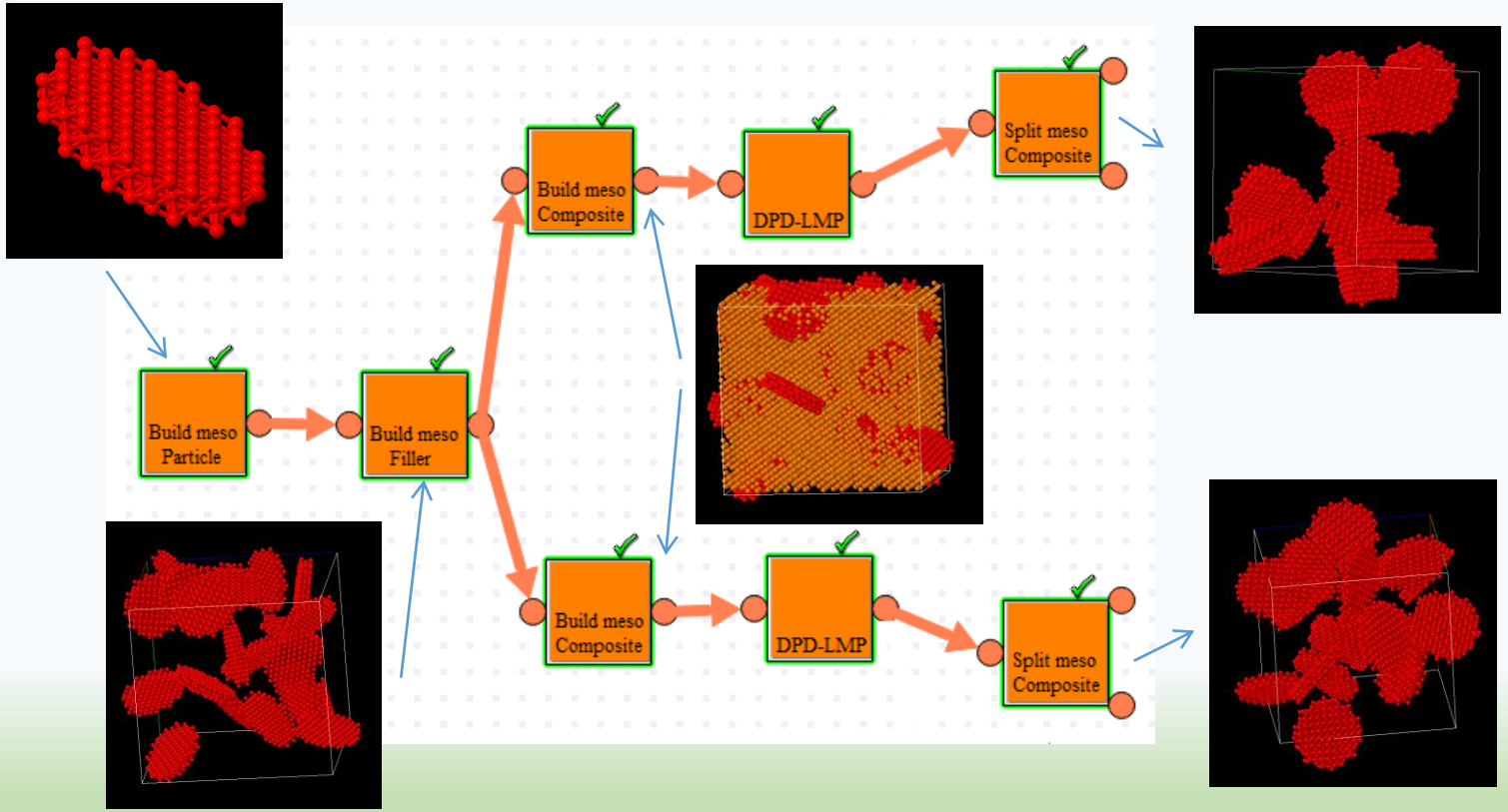
**Clay-filled polymer composites were obtained in the 1990s**.

- They have improved mechanical properties.
- The properties depend on the dispersion of the filler in the matrix.
- Interest in them continues to this day, and it is common to consider them using multilevel approaches.



# relaxation of structures and distribution of filler

Different parameters of the interaction between the matrix and the filler lead to different distribution of the filler in the matrix.




Filler particles are repelled weaker from each other than from the matrix:
**Filler aggregation**

Filler particles are repelled more strongly from each other than from the matrix.
**Homogeneous distribution**

**It is possible to predict the distribution of the filler depending on its interaction with the matrix**

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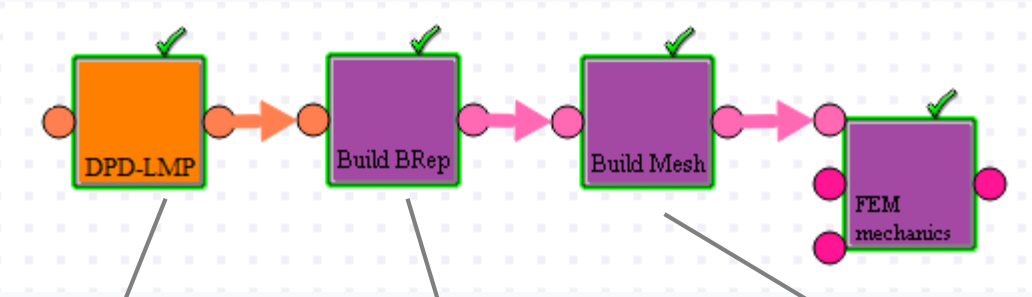
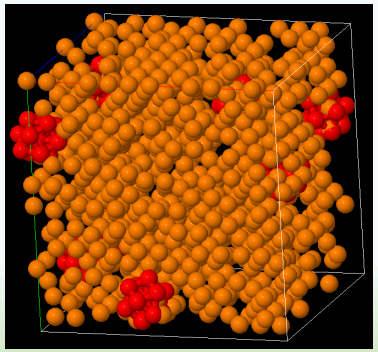
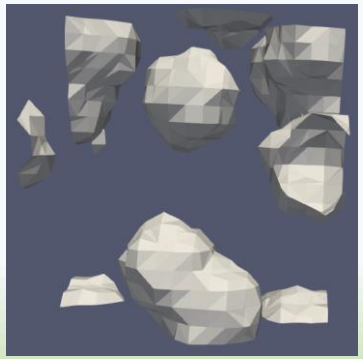
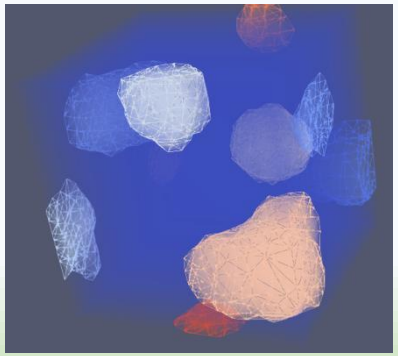
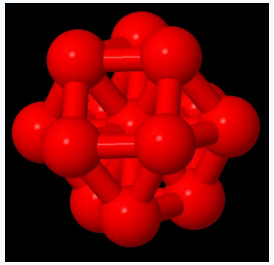
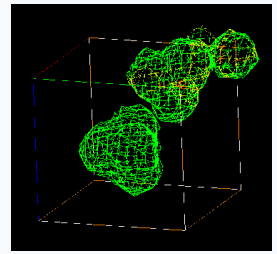
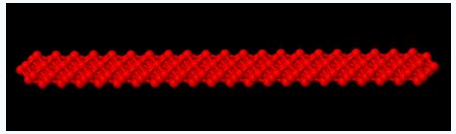
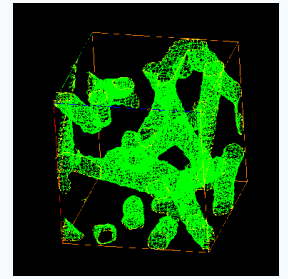
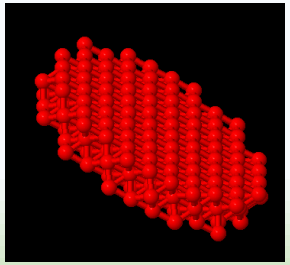
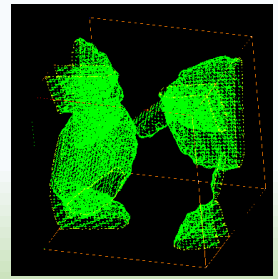
# transition from mesoscale to macro level

1. Creates a surface mesh based on the mesoscale structure.
2. Building a volumetric mesh.
3. Calculation on the constructed volumetric mesh.




elastic tensor

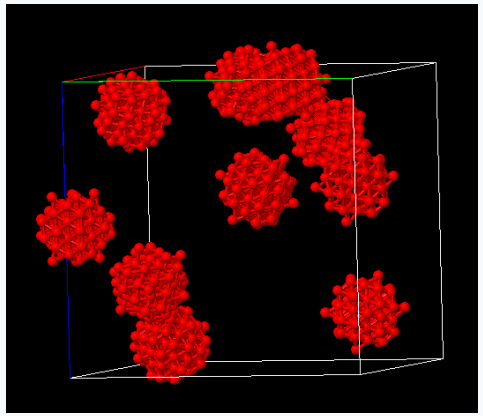










The procedure for the transition to the macro level is fully automated and universal for any form of filler

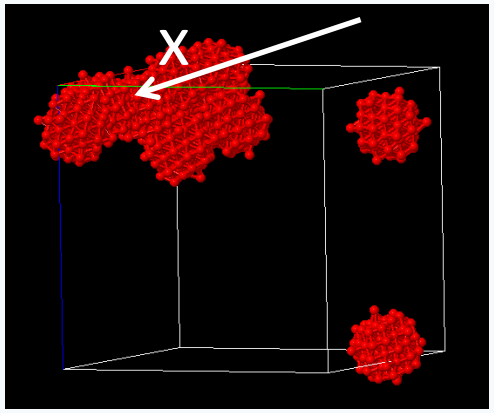
1 - Lorensen W. E., Cline H. E. Marching cubes: A high resolution 3D surface construction algorithm //ACM siggraph computer graphics. – 1987. – Т. 21. – №. 4. – С. 163-169

# calculation of the mechanical properties of a composite filled with spherical particles

Different distributions of the filler lead to different values of the elastic moduli at the same volumetric concentration of the filler, as well as anisotropy of properties. With percolation, the rigidity of the system in this direction increases significantly.

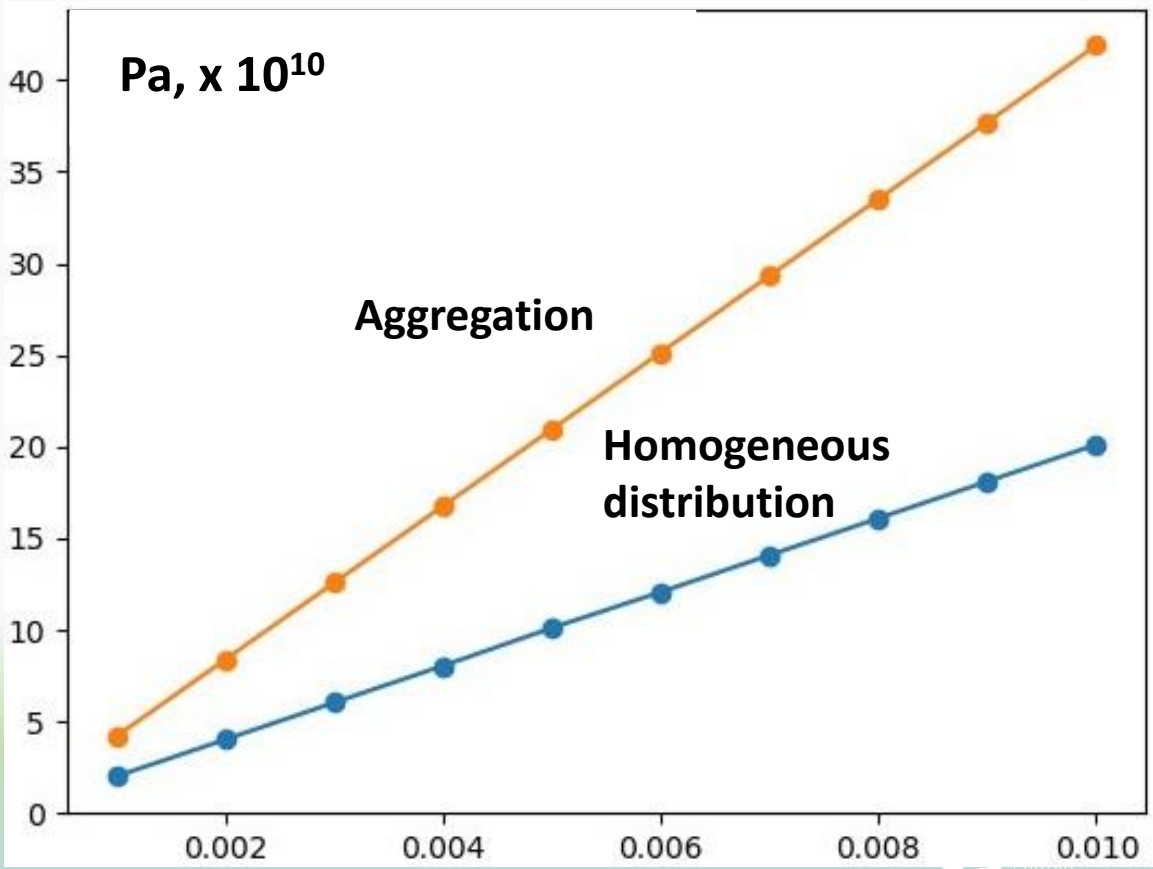


**Aggregation**
E = 4.2 GPa




**Homogeneous distribution**
(percolation along - x)
$E_x$ =11 GPa

**Dependence of stresses on deformation (along x, direction of percolation in one of the structures)**




**Data transfer for structure conversion and calculation of effective properties at the macro level are carried out automatically.**

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# conclusion

- The **MULTICOMP** software package enables predictive calculations of the properties of polymer matrix nanocomposites based on multilevel modeling, including:
  - Determination of the structure of composites, distribution of the filler in the matrix
  - Determination of Effective Macroscopic Properties of the Whole Composite
- The **MULTICOMP** package allows you to create flexible calculation scenarios using high-performance computing resources, providing automatic data transfer and control over the execution of calculations
- The **MULTICOMP** package can be used both for the practical development of new materials and for teaching students methods of computational materials science.
- The **MULTICOMP** software package is an open platform that implements the ***Scientific Workflow*** concept and allows users to create their own calculation scenarios and add new calculation modules

# areas of practical application MULTICOMP

- Predicting the properties of polymer matrices depending on the chemical structure of monomers
- Prediction of changes in the glass transition temperature of a polymer matrix upon the introduction of a nanoscale filler
- Predicting changes in the mechanical properties of polymer matrices upon the introduction of a nanoscale filler (hardening of plastic, changing the properties of rubber products)
- Predicting changes in the thermal conductivity of polymer matrices upon the introduction of a nanoscale filler (insulating materials, membranes)
- Predicting changes in the gas permeability of polymer matrices upon the introduction of a nanoscale filler (film, membrane)

# application of MULTICOMP in education

- The developed package can be used both for the practical development of new materials and for teaching students methods of computational materials science.
- With the help of **MULTICOMP**, students can master the basics of atomistic and mesoscopic modeling of polymer systems without the need to study specific modeling programs and direct work with remote computing resources (creating computer classes)
- Based on **MULTICOMP**, laboratory workshops can be developed for the introduction of composite materials based on polymer matrices with organic and inorganic fillers into physics and chemistry.
- Also, this Package can be useful for teaching the basics of multilevel modeling of composite materials (end-to-end modeling from atomistics to the macrolevel)

# thank you for the attention

## Acknowledgment

This work was carried out using high-performance computing resources of federal center for collective usage at NRC "Kurchatov Institute" (http://computing.kiae.ru/) and a software package for multi-level predictive modeling morphology, thermal and mechanical properties of nanocomposites with polymer matrix, developed in the framework of the project ERA-RUS-14891 (0021028) by Kintech Lab Ltd (http://www.kintechlab.com/).

**The Russian Foundation for Basic Research (RFBR) (project 16-03-00223) is also appreciated.**

РОССИЙСКАЯ ФЕДЕРАЦИЯ

СВИДЕТЕЛЬСТВО

о государственной регистрации программы для ЭВМ

№ 2018615740

Multicomp

Правообладатель: *Общество с ограниченной ответственностью «Лаборатория Кинтех» (RU)*

Авторы: *см. на обороте*

Заявка № 2018613030
Дата поступления 28 марта 2018 г.
Дата государственной регистрации
в Реестре программ для ЭВМ *15 мая 2018 г.*

*Руководитель Федеральной службы по интеллектуальной собственности*

*Г.П. Ивлиев*

KINTECH LABORATORY

**Contact us**: Kintech Lab Ltd. http://www.kintechlab.com
support@kintech.ru : for general service and product information
info@kintech.ru: for all questions concerning Kintech Lab software

# БЛАГОДАРНОСТИ

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- с использованием высокопроизводительных вычислительных ресурсов:
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  - суперкомпьютерного комплекса Московского государственного университета имени М.В. Ломоносова

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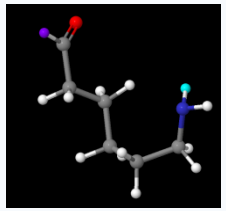
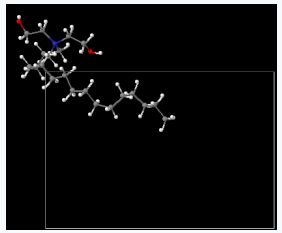
  info@kintech.ru : для связи по остальным вопросам
- WWW
  http://www.kintechlab.com/ru

# calculation of mechanical properties of organomodified montmorillonite intercalated with polyamide-6

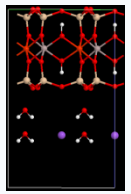
## Layered composite construction procedure



comonomer (CVFF)

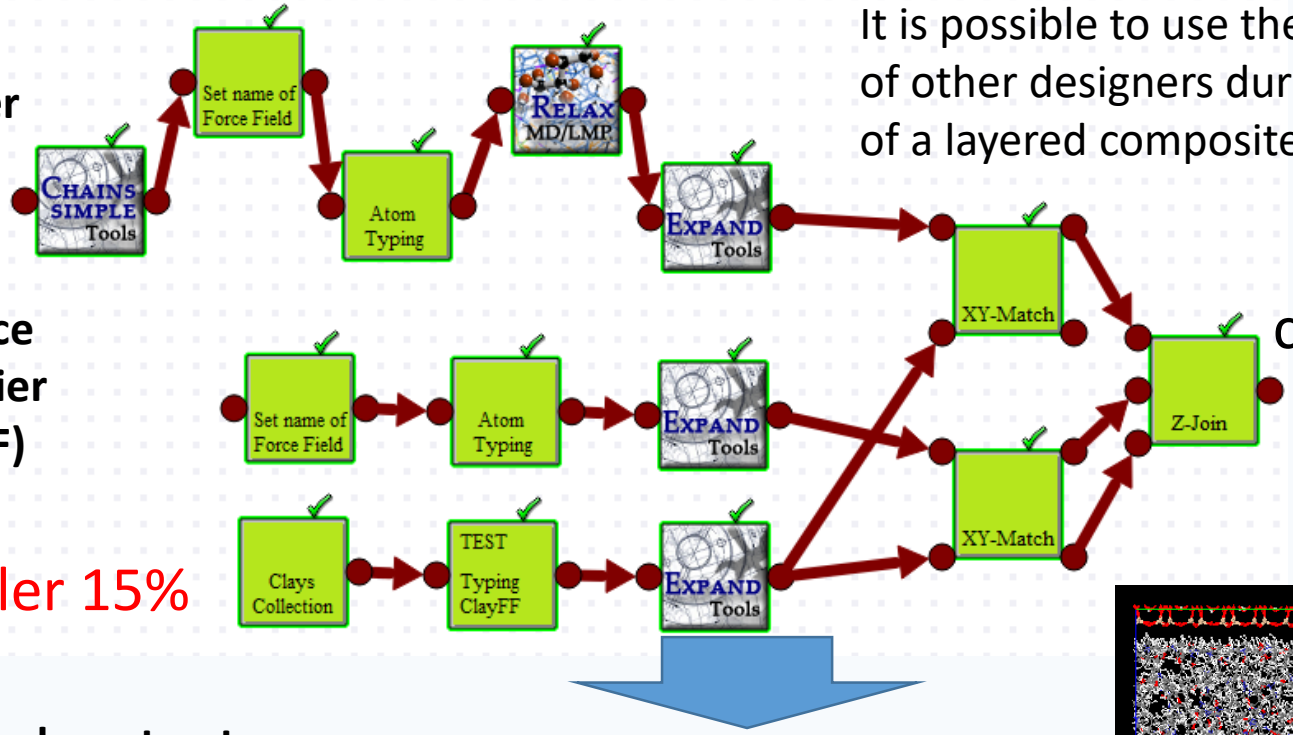


surface modifier (CVFF)



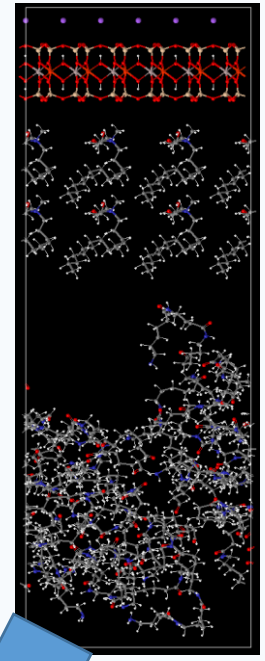
filler (ClayFF)

filler 15%

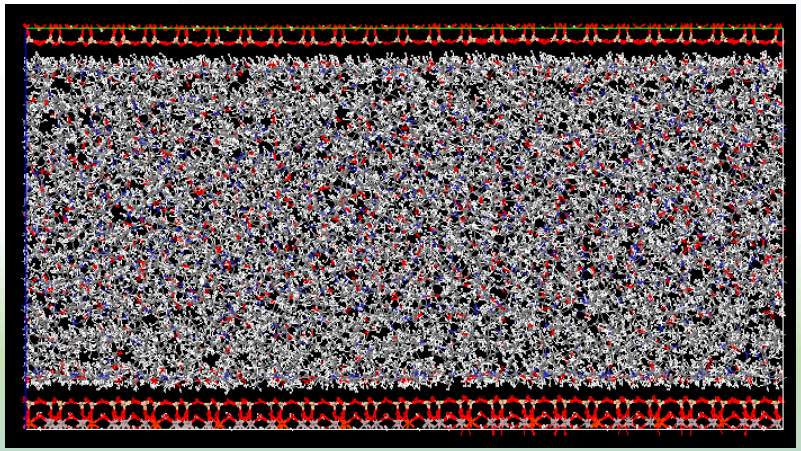



It is possible to use the results of the work of other designers during the construction of a layered composite

3 phase composite



relaxation



**To build composites based on structures with different frequency:**

- Construction of each of the structures (each with its own parameterization).
- Coercion to the same planar dimensions Combination of structures.

**Elastic moduli obtained by calculation:**

EPA6 = 2.8 Gpa

EMMT = 232 Gpa

Ecomposite = 41 GPa

Skomorokhov A. S., Knizhnik A. A., Potapkin B. V. //The Journal of Physical Chemistry B. – 2019. – Т. 123. – №. 12. – С. 2710-2718.