Russian Supercomputing Days

KINTECH LABORATORY

ИНЭОС

ВИНИТИ

September 29-30, 2025, Moscow

Thermal conductivity calculations in the MULTICOMP package

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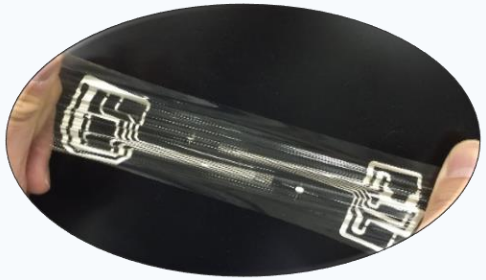
The work is performed on the basis of Kintech Lab Ltd.

polymer based materials: applications

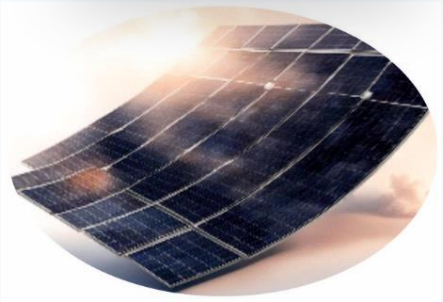


Flexible electronics

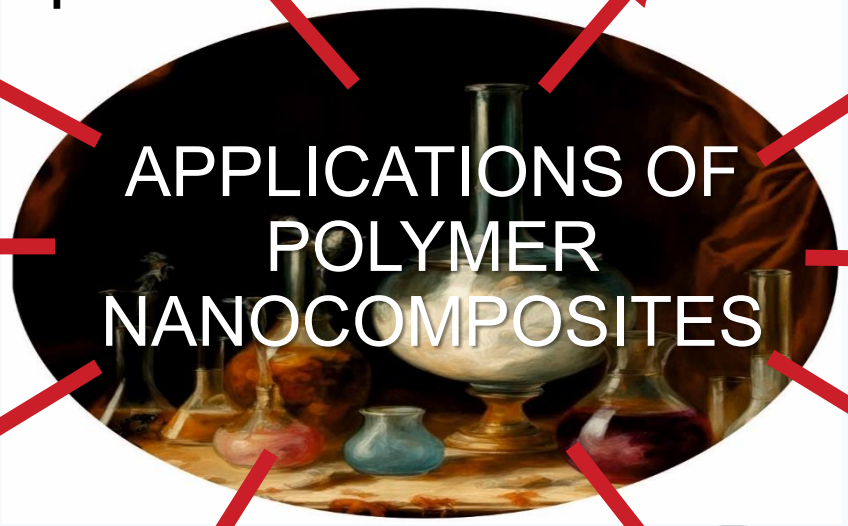
LCD panels

Medical

Gels



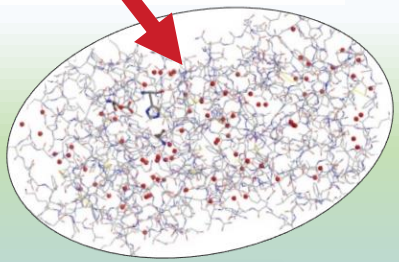
Organic photovoltaics



Glues / paints

Chemical fibers

Transport



Syntetic catalysts

Packaging

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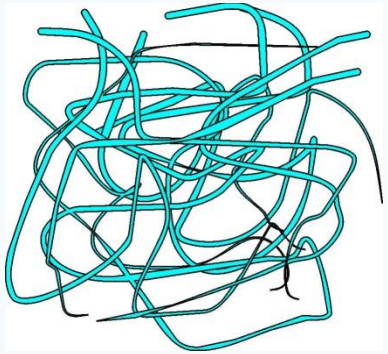
polymer nanocomposites

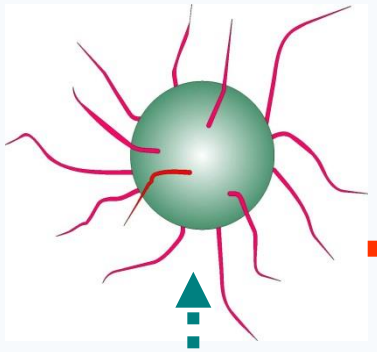
Combination of a polymer matrix and filler that have at least one dimension (i.e. length, width, or thickness) in the nanometer size range (1 nm = 10^{-9} m)

- **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.

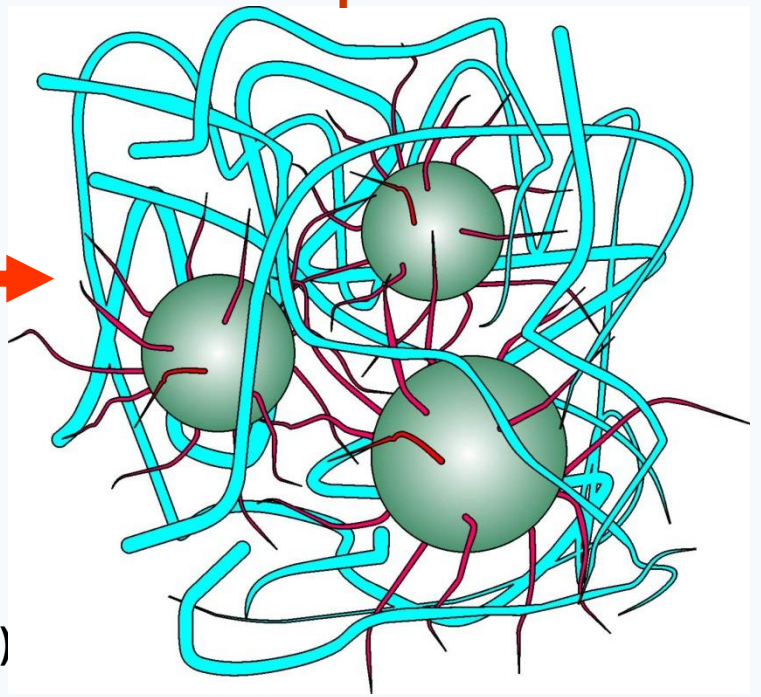
Matrix



Fillers



Composite



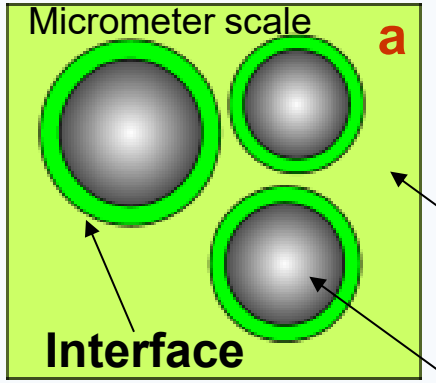
Surface Modifiers

-OH

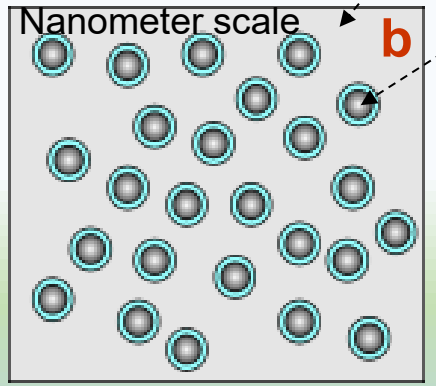
$-[SiH_2-O-]_n-H$

Etc.

Nanoparticles (3D)
Nanosheets/Flakes (2D)
Thread/fiber/nonowires (1D)

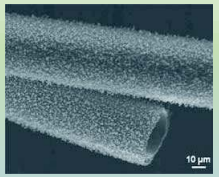


$V_{interface}/V_{filler} < 1$

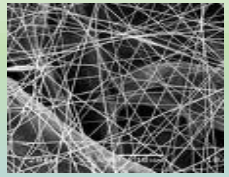


$V_{interface}/V_{filler} \sim 1$

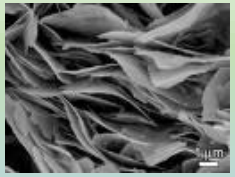
C tubules



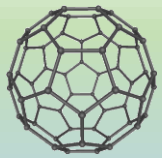
Glass fibers



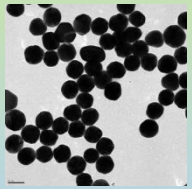
Clay



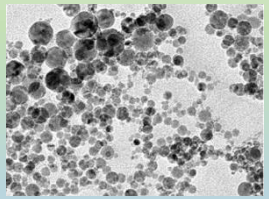
Fullerenes



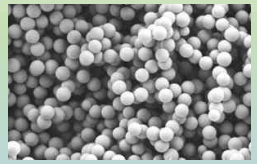
Au



TiO_2



SiO_2



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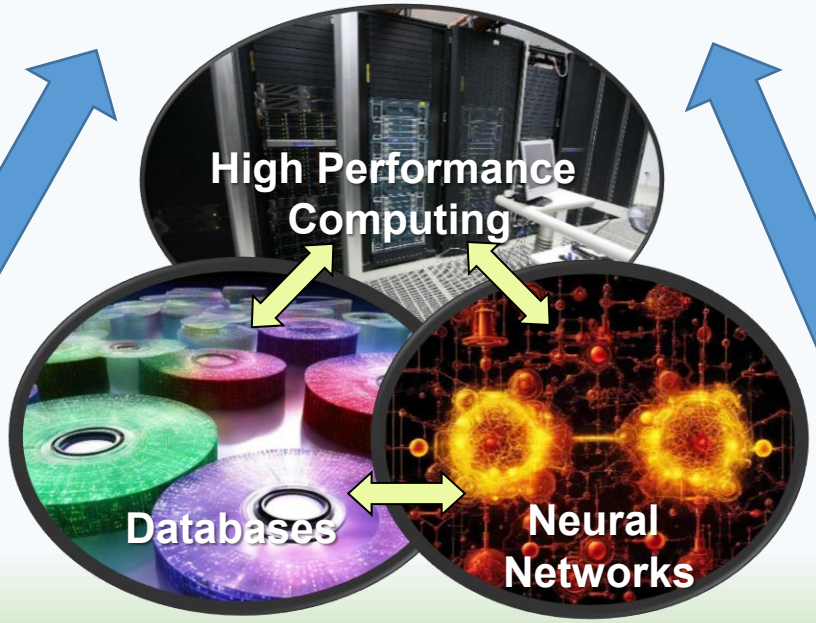
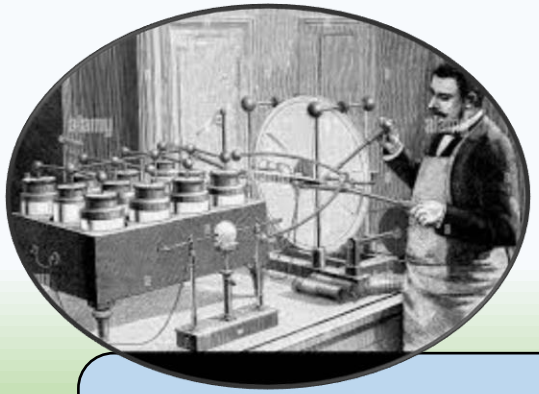
Computer modeling in the development of new materials

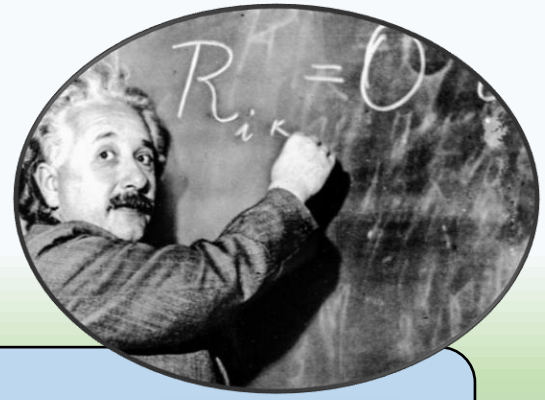
INPUT:
Chemical structure
environment parameters

COMPUTER MODELING

OUTPUT:
Structural, physical & chemical properties



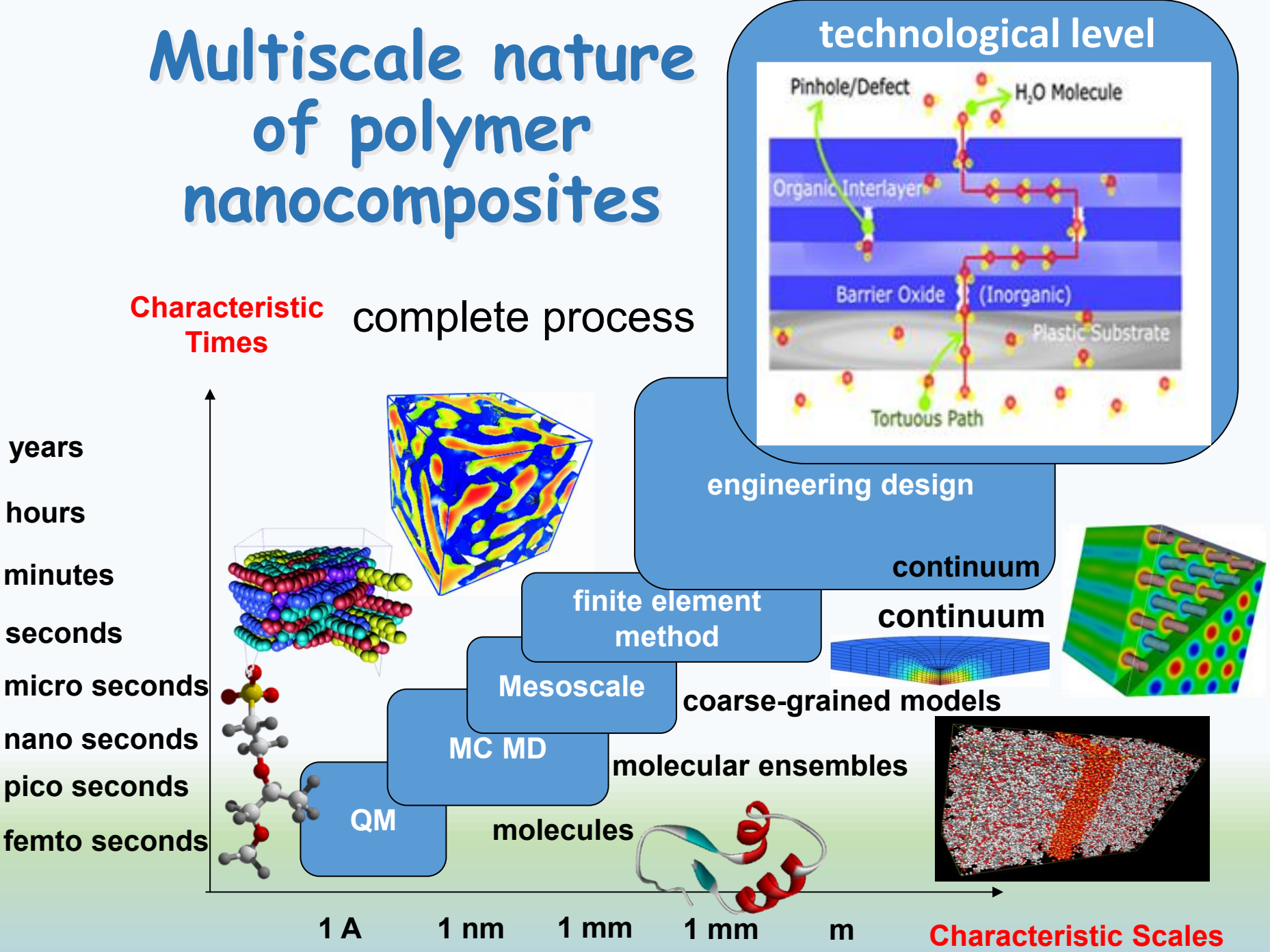




EXPERIMENT

THEORY

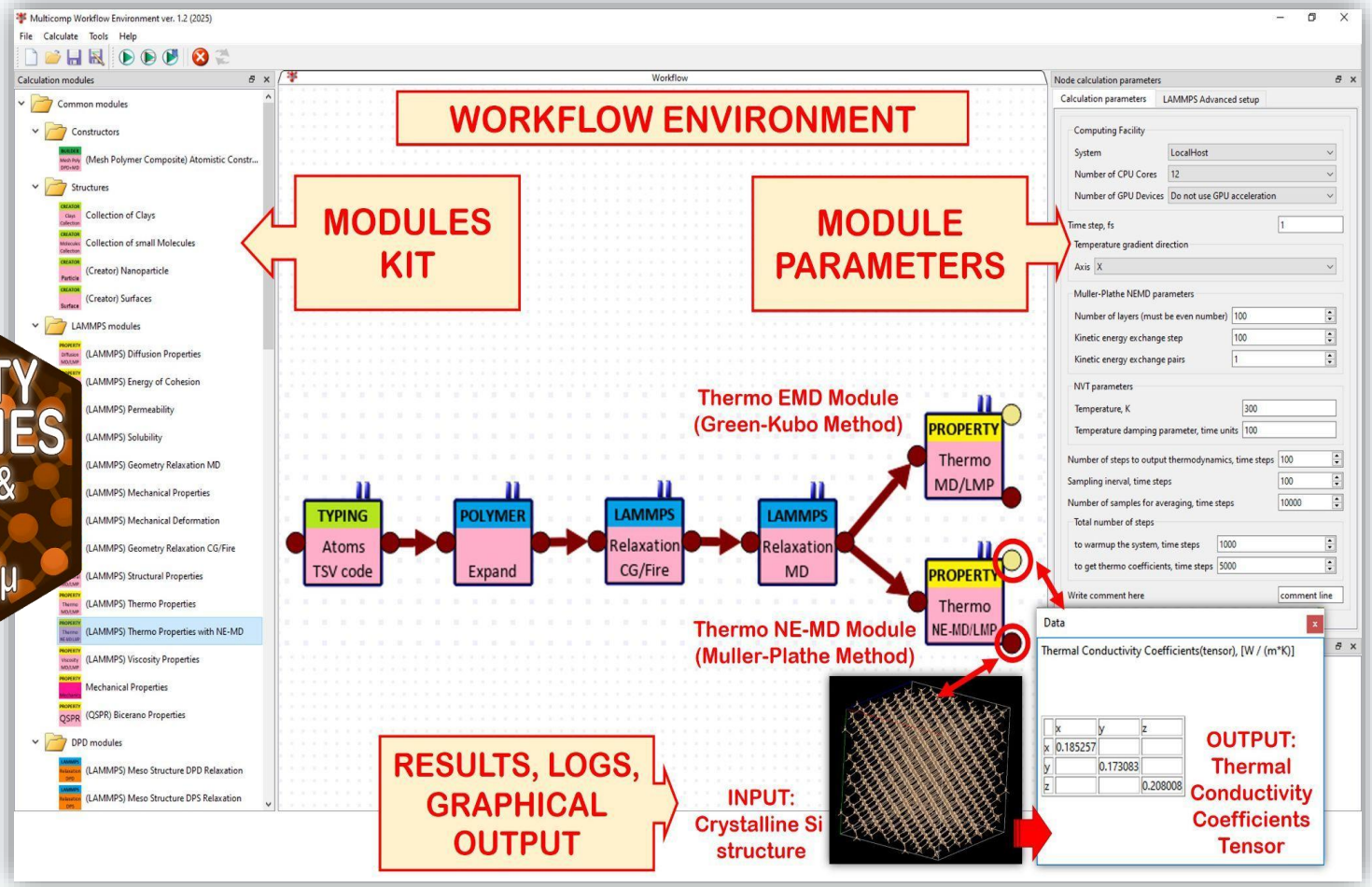
Multiscale nature of polymer nanocomposites



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

Graphical User Interface: scientific workflow approach



The modeling process is divided into separate modules at a fixed level of the spatial and time scale hierarchy

CHEMICAL COMPOSITION

MATERIAL MODEL

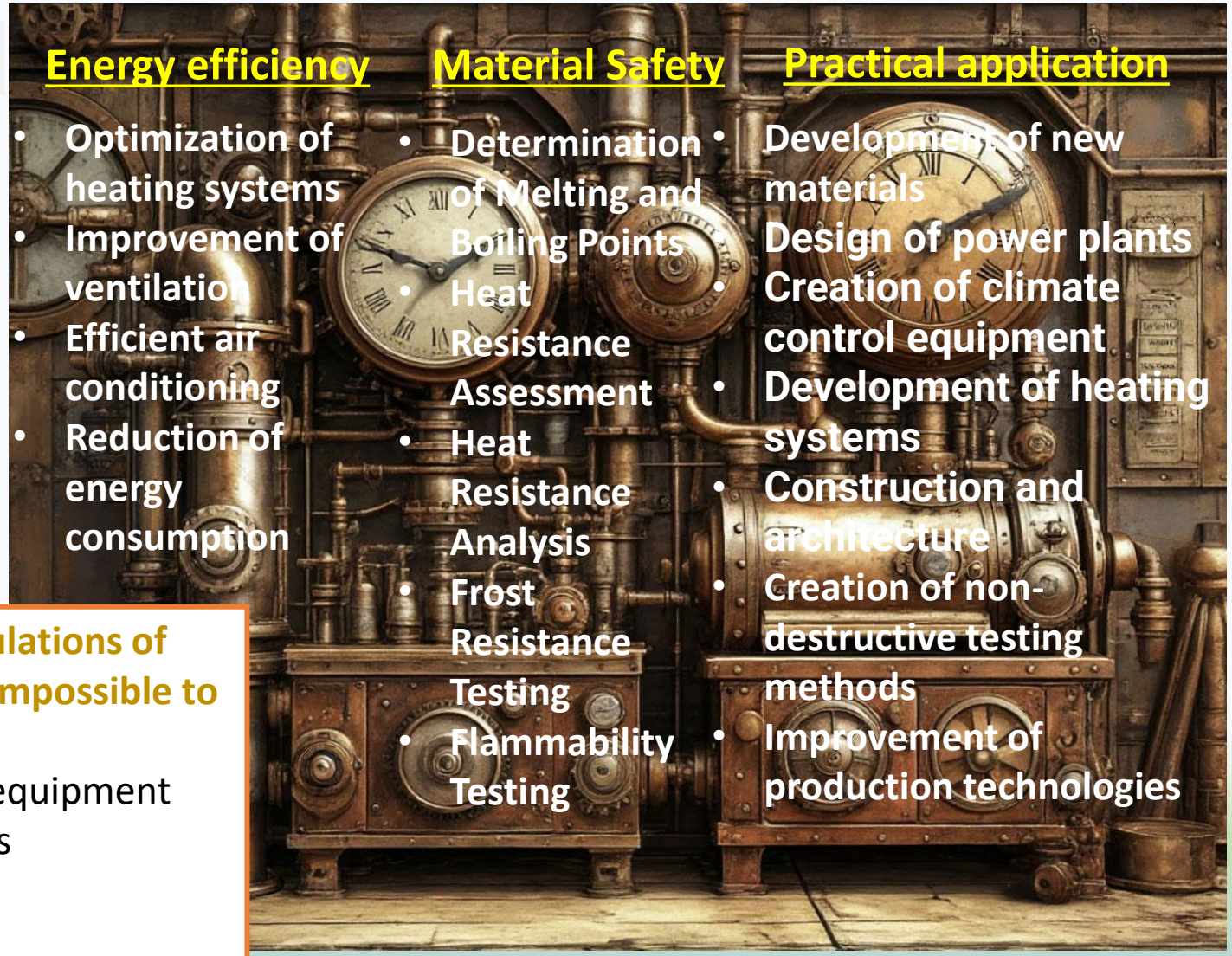
PHYSICAL PROPERTIES

MULTICOMP

The importance of the thermal properties of materials

Performance characteristics

- **Determination of the behavior of materials at different temperatures**
- **Assessment of the ability to accumulate heat**
- **Analysis of the possibilities of heat removal**



Energy efficiency

- Optimization of heating systems
- Improvement of ventilation
- Efficient air conditioning
- Reduction of energy consumption

Material Safety

- Determination of Melting and Boiling Points
- Heat Resistance Assessment
- Heat Resistance Analysis
- Frost Resistance Testing
- Flammability Testing

Practical application

- Development of new materials
- Design of power plants
- Creation of climate control equipment
- Development of heating systems
- Construction and architecture
- Creation of non-destructive testing methods
- Improvement of production technologies

Economic aspects

- Study of properties of existing materials and optimization of material costs
- Reduction of heat energy losses
- Increasing energy efficiency
- Reduction of environmental impact

Without precise calculations of thermal properties it is impossible to ensure:

- Reliable operation of equipment
- Durability of structures
- Operational safety
- Economic efficiency

Equilibrium molecular dynamics (EMD) for computing thermal conductivity

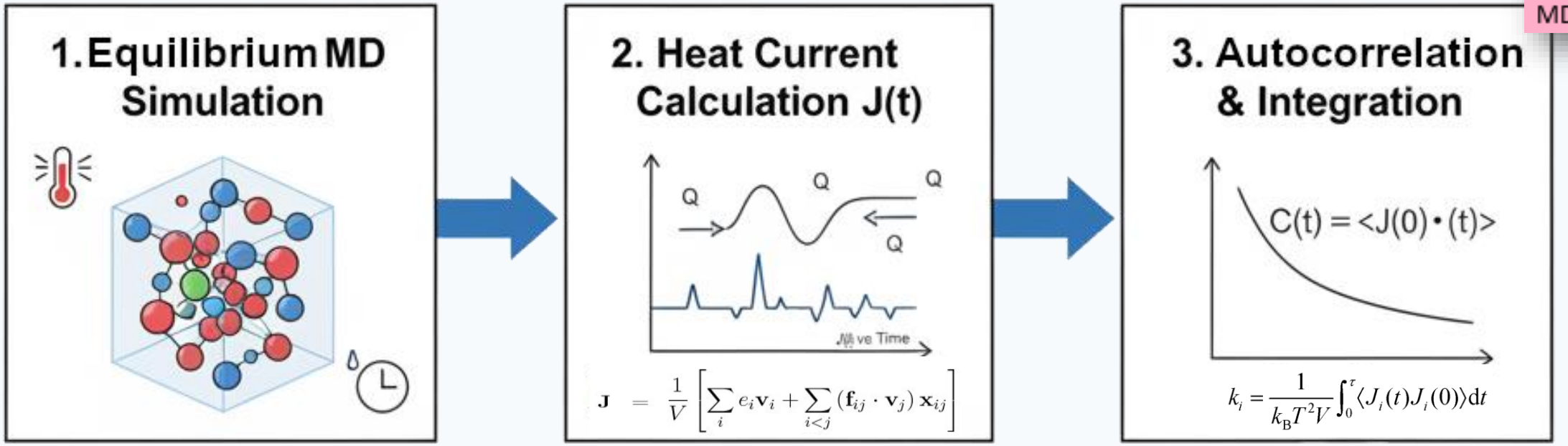
Thermal conductivity is calculated a consequence of the fluctuation-dissipation theorem based on the equilibrium current-current autocorrelation function of heat flux calculated at chosen timesteps of the MD simulation run (Green-Kubo* formula).

PROPERTY

Thermo

MD/LMP

✓



✓ computationally efficient for bulk materials, homogeneous systems and small simulation domains.

✓ can reproduce intrinsic material properties without directly imposing the temperature gradient in the system

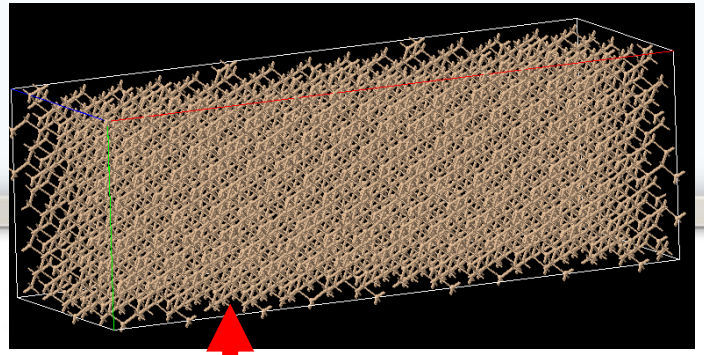
✓ does not suffer from the boundary and finite-size effects inherent in non-equilibrium methods

➢ sufficient convergence of the current-current autocorrelation function requires very long simulation times, especially for materials with high thermal conductivity

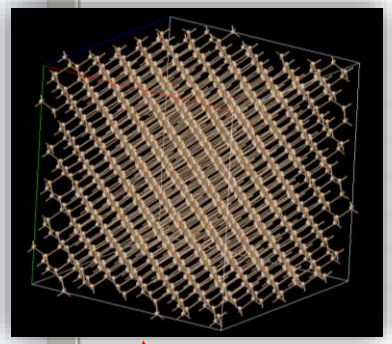
➢ less effective for systems with strong anharmonicity or complex interfaces

** Kubo, R. Journal of the physical society of Japan 12.6 (1957): 570-586.*

Case study: thermal conductivity of Si crystal with different sizes



Change size of the crystalline Si structure



Thermo EMD Module (Green-Kubo Method)

Thermo NE-MD Module (Muller-Plathe Method)

INPUT: Crystalline Si structure

OUTPUT: Thermal Conductivity Coefficients Tensor

Calculating the thermal conductivity of crystalline silicon: EMD simulations

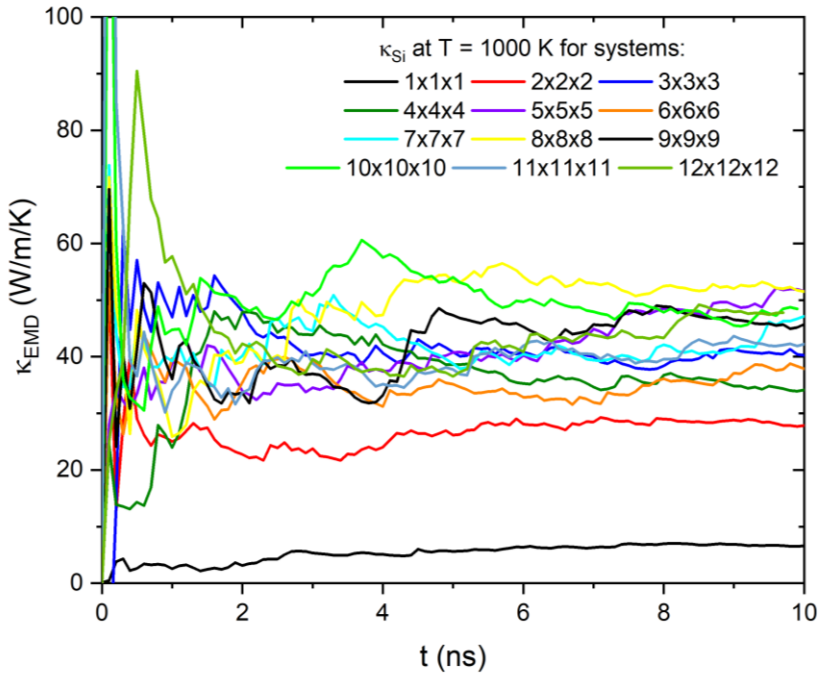
- **Equilibrium molecular dynamics (EMD):** In our calculation, we wanted to investigate both the finite simulation size effects and the effects related to the autocorrelation estimations from the obtained statistical data.

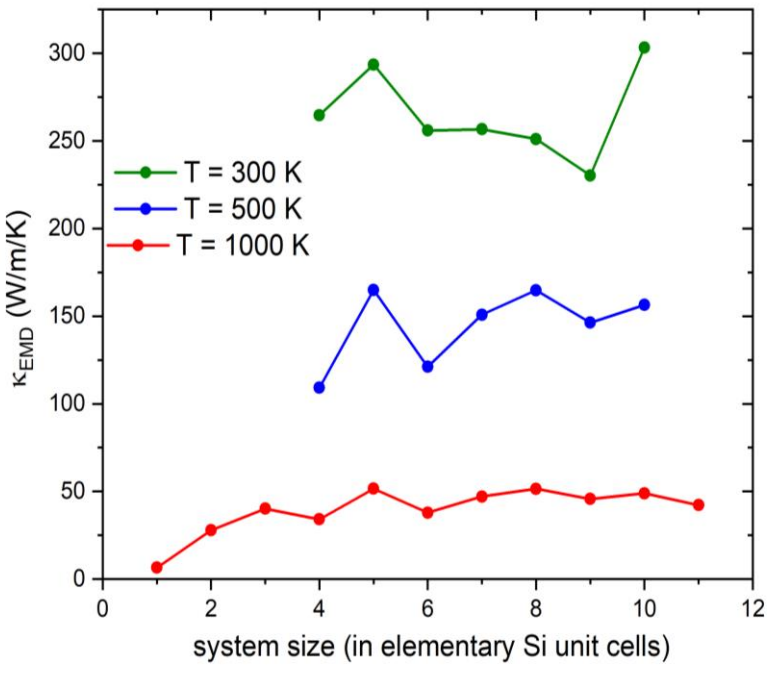
PROPERTY
Thermo
MD/LMP

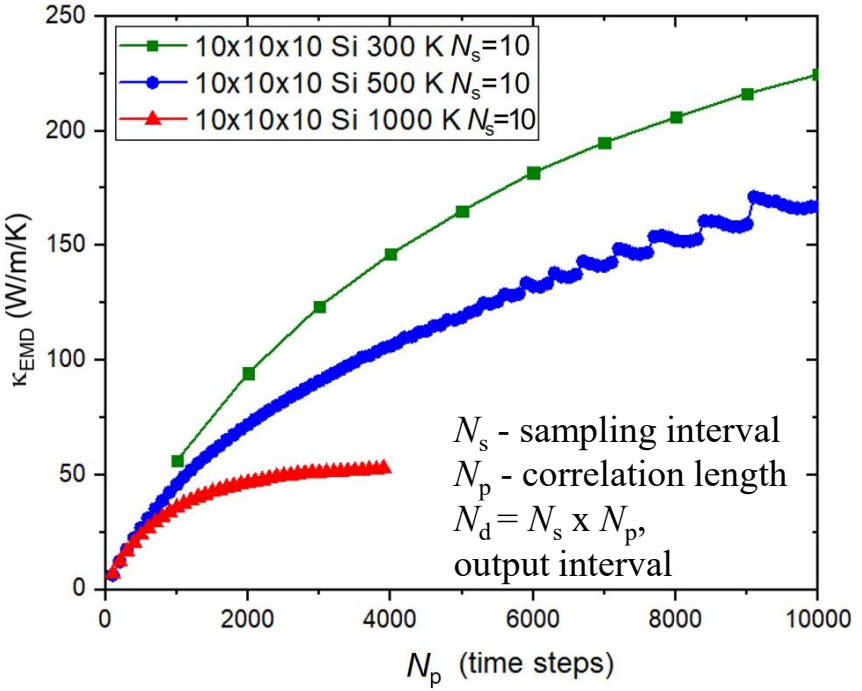
CONVERGENCE TIME:
equilibration can require a significant simulation time of 10 ns

SIZE EFFECTS:
reasonable convergence requires systems with 5x5x5 silicon unit cells in all directions (1000 atoms)

AUTOCORRELATION EFFECTS:
Significant effects due to the averaging parameters of the autocorrelation function





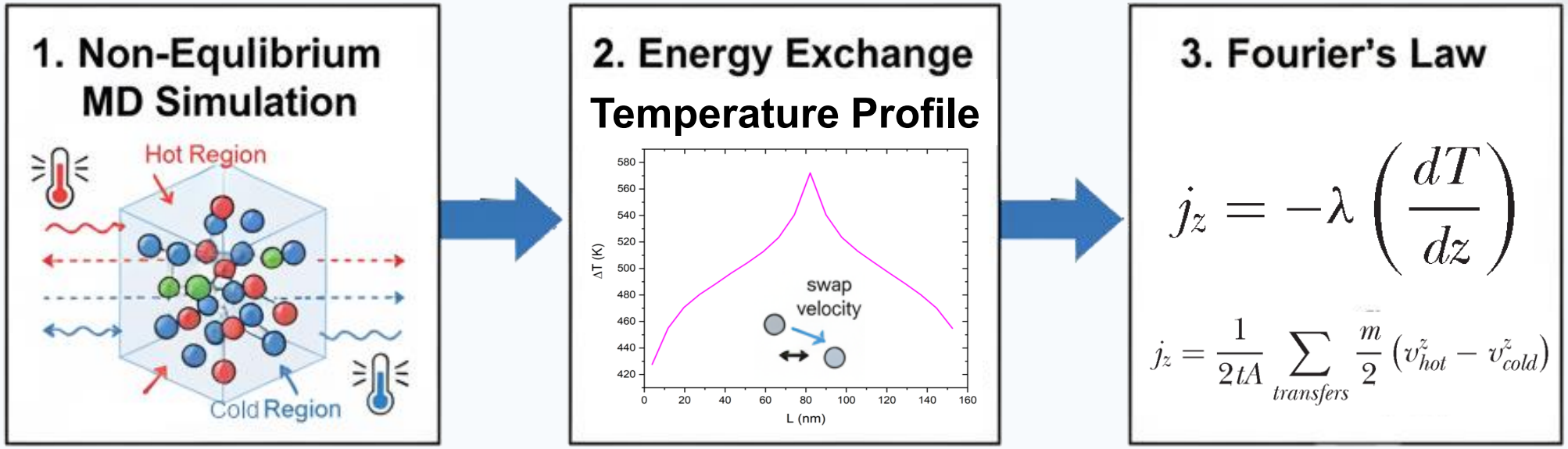


✓ **Similar results were observed in the study by Shelling et al [Physical Review B, 65(14), 144306. (2002)]**

Nonequilibrium molecular dynamics (NEMD) for computing thermal conductivity

Müller-Plathe method** imposes a heat flux by exchanging velocities between cold and hot atoms. Over time, these energy exchanges create a temperature gradient in the system that can be used to calculate thermal conductivity as the ratio of the heat flux to the temperature gradient.

PROPERTY
Thermo
NE-MD/LMP



- ✓ relatively fast convergence and direct control of the heat flux
- ✓ suitable for systems with strong anharmonicity or interfaces: preferable for calculating thermal resistance, for example, between the filler and the polymer matrix, or in other anisotropic materials

- ➢ calculations are sensitive to boundary effects as well as to the choice of simulation parameters (such as system size, heat exchange frequency, and layer definitions)
- ➢ does not directly provide intrinsic material properties like EMD, but rather an effective thermal conductivity that depends on the imposed gradient

*** Müller-Plathe, F. Phys Rev E Stat Phys Plasmas Fluids Relat Interdiscip Topics 1999, 59 (5 Pt A), 4894–4898.*

Calculating the thermal conductivity of crystalline silicon: NEMD simulations

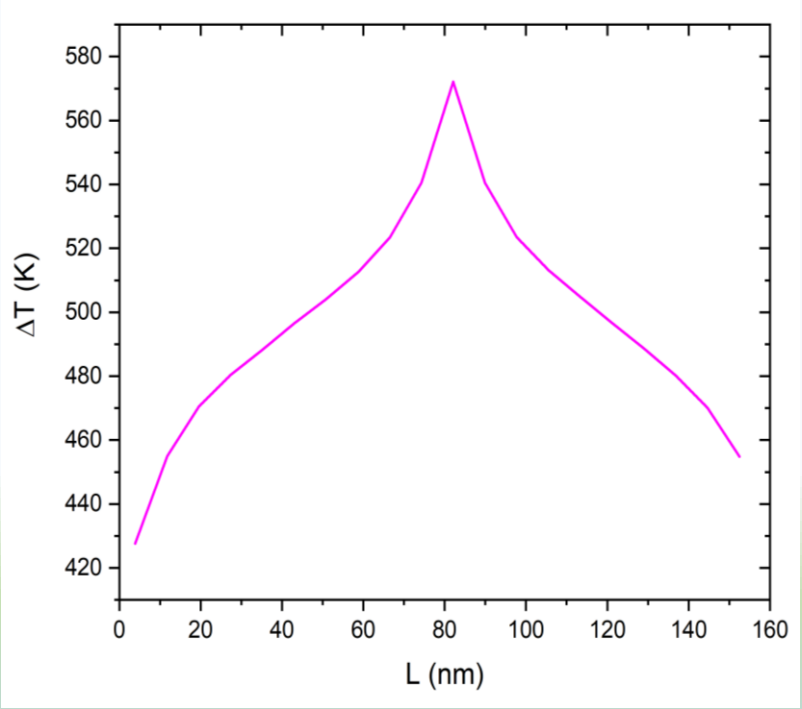
- **Nonequilibrium molecular dynamics (NEMD):** For the verification of the "**ThermoProperties NE-MD**" module, crystalline silicon was studied at 500 K with a focus on finite-size effects.

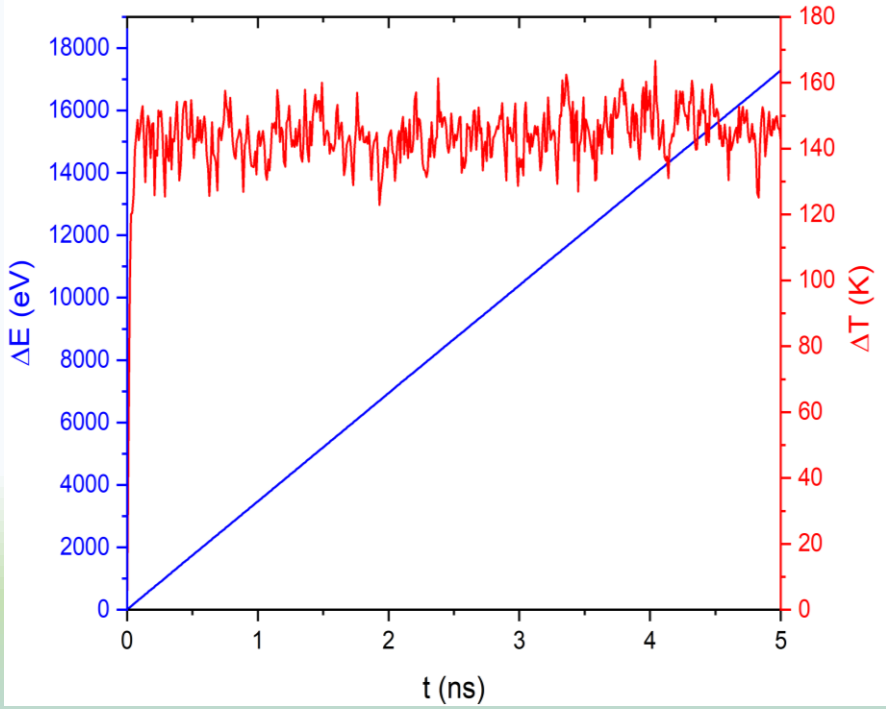
PROPERTY
Thermo
NE-MD/LMP

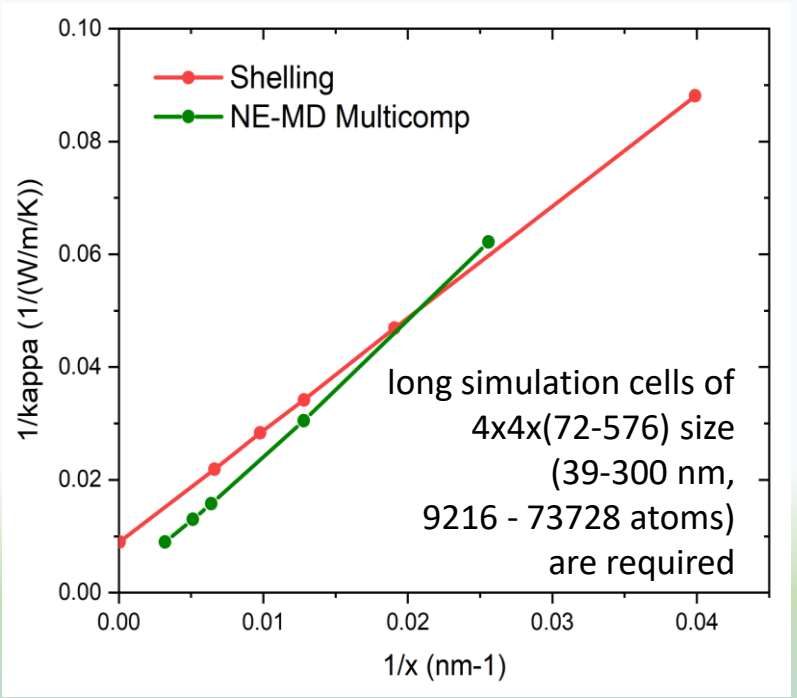
NON-EQUILIBRIUM SYSTEM:
time-averaged temperature profile determined in the system

CONVERGENCE TIME:
require smaller simulation time of less than 1 ns

SIZE EFFECTS:
system sizes comparable to or larger than the phonon mean free path (L_z >> λ) are required for accurate results







✓ **Module verified with respect to the study by Shelling et al [Physical Review B, 65(14), 144306. (2002)]**

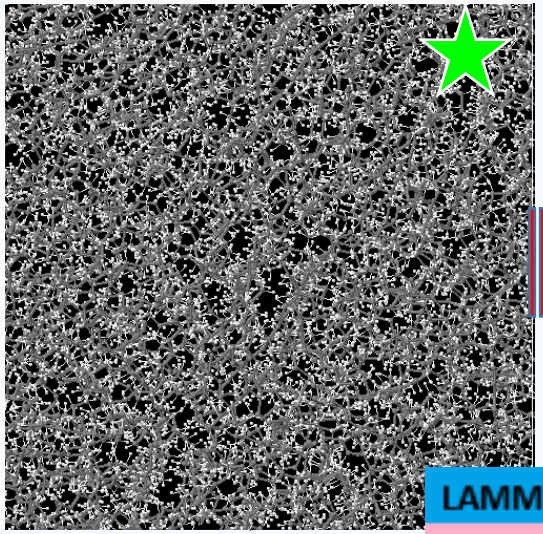
Comparison of atomic-level simulation methods for computing thermal conductivity of crystalline silicon in the MULTICOMP Package

Method	Crystalline Silicon Thermal Conductivity κ (W/m/K)		
	T = 300 K	T = 500 K	T = 1000 K
Simulation / EMD Stillinger-Weber potential (PROPERTY: Thermo MD/LMP)	**220-290 [this study]** 170-240 [1,2,3,4]	**130-150 [this study]**	**50-60 [this study]** 62-66 [5]
Simulation / NEMD Stillinger-Weber potential (PROPERTY: Thermo NE-MD/LMP)	**180-200 [this study]** 205 [4]	**110-150 [this study]** 100-120 [5]	
Experiment	160-240 [6,7]	80 [6]	50 [6]

- ✓ **The modeling results are in quantitative and qualitative agreement with the experimental data and previous MD simulations based on EMD and NEMD approaches**
- ✓ **The results summarized in this table clearly show that for crystalline silicon, both implemented EMD and NE-MD-based methods give the same result within the method error.**

1 Poetzsch, R. H., & Böttger, H. (1994) Physical Review B, 50(21), 15757. 2 Fang, K. C., Weng, C. I., & Ju, S. P. (2006). Nano-technology, 17(15), 3909.
3 Yang, L., Yang, N., & Li, B. (2014) Nano letters, 14(4), 1734-1738. 4 Park, M., Lee, I. H., & Kim, Y. S. (2014) Journal of Applied Physics, 116(4).
5 Schelling, P. K., Phillpot, S. R., & Keblinski, P. (2002). Comparison of atomic-level simula-tion methods for computing thermal conductivity. Physical Review B, 65(14), 144306
6 Capinski, W. S., Maris, H. J., Bauser, E., Silier, I., Asen-Palmer, M., Ruf, T., ... & Gmelin, E. (1997) Applied physics letters, 71(15), 2109-2111.
7 Ruf, T., Henn, R. W., Asen-Palmer, M., Gmelin, E., Cardona, M., Pohl, H. J., ... & Senni-kov, P. G. (2000) Solid State Communications, 115(5), 243-247

An example where NEMD works more efficient then EMD

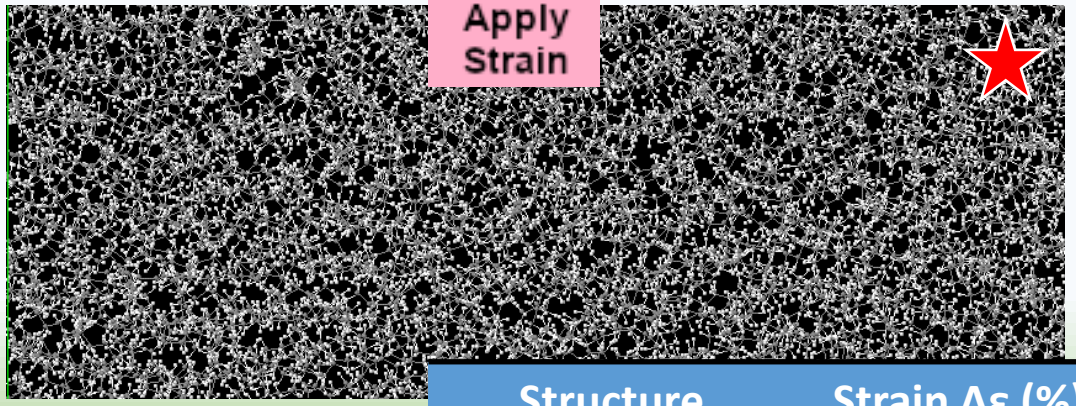


POLYETHYLENE (PE) SYSTEM ~10000 atoms

Constant volume stretching X2 (100% strain)

PROPERTY
Thermo
NE-MD/LMP

LAMMPS
Apply Strain



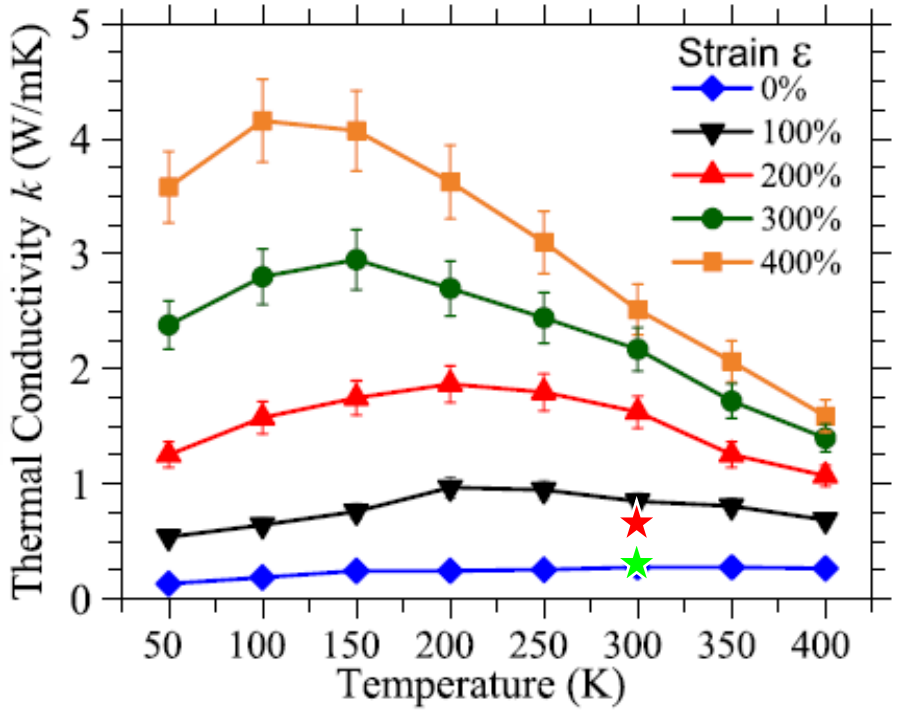


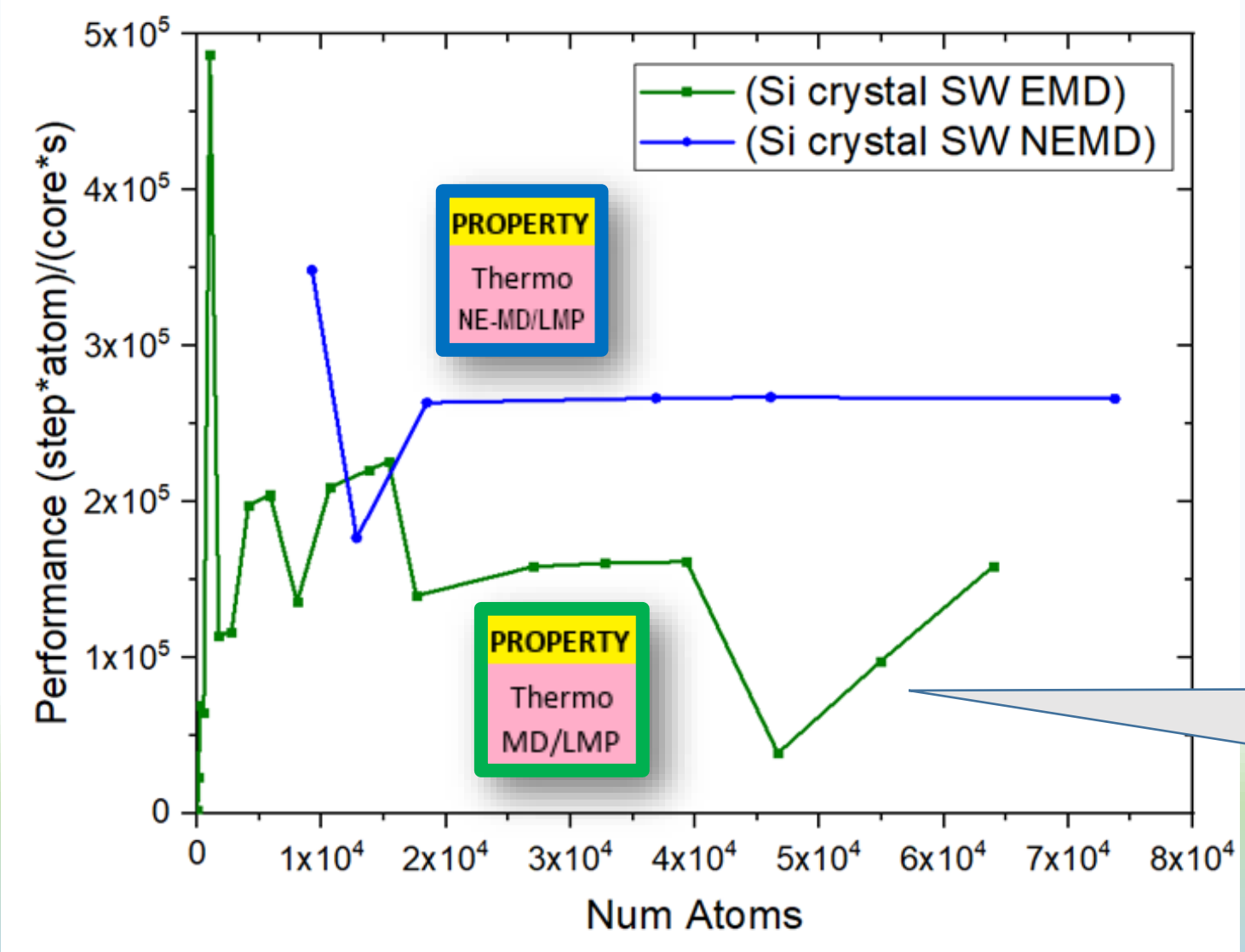
FIG. 3. Variation of thermal conductivity of amorphous polyethylene with temperature at different strains.

R. Muthaiah and J. Garg
J. Appl. Phys. 124, 105102 (2018)

Structure	Strain Δε (%)	κ_{PE}^{0} (W/m/k)	Nematic order S
Polyethylene PE	0	0.17	0
	100	0.39	0.61

Performance comparison for EMD and NEMD simulation methods

The presented characteristic (step × atom) / (CPU core × second) quantifies the performance of molecular dynamics simulations by measuring the number of atom-steps computed per second per CPU core.



Intel Xeon E5 2680 (CPU)
16 hours real time for 1 ns MD run for 70,000 atoms
Performance ~ 10^5 (step × atom) / (GPU Compute Units × second)

NVIDIA GeForce RTX 4090 (GPGPU):
1 hours real time for 1 ns MD run for 120,000 atoms.
Performance ~ 10^3 (step × atom) / (GPU Compute Units × second)

The NE-MD module demonstrates approximately x2 faster convergence compared to EMD due to its more efficient heat transport characterization

Conclusions

- Thermal conductivity of crystalline silicon was evaluated using EMD and NEMD molecular dynamics approaches available in the current release of the MULTICOMP package
- The consistency between EMD- and NEMD-based calculations provides a robust validation of the computational approach and confirms the reliability of the previously developed EMD-based "ThermoProperties" module and serves as a verification of the newly introduced NEMD-based "ThermoProperties NE-MD" module
- EMD and NEMD methods complement each other and offer specific advantages depending on the system under study. New functionalities for the evaluation of thermophysical properties make MULTICOMP a unique and comprehensive platform for the design of high-performance polymer nanocomposites.

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Acknowledgments


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
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Руководитель Федеральной службы по интеллектуальной собственности

Г.П. Ивлиев

Данная работа выполнена:

- с использованием высокопроизводительных вычислительных ресурсов:
  - федерального центра коллективного пользования в НИЦ «Курчатовский институт», http://computing.kiae.ru/
  - суперкомпьютерного комплекса Московского государственного университета имени М.В. Ломоносова

input

- Chemical structure of components
- Geometry of nanoparticles and their properties
- Weight ratio of components
- Temperature, pressure and etc.

output

Physical properties of the material:

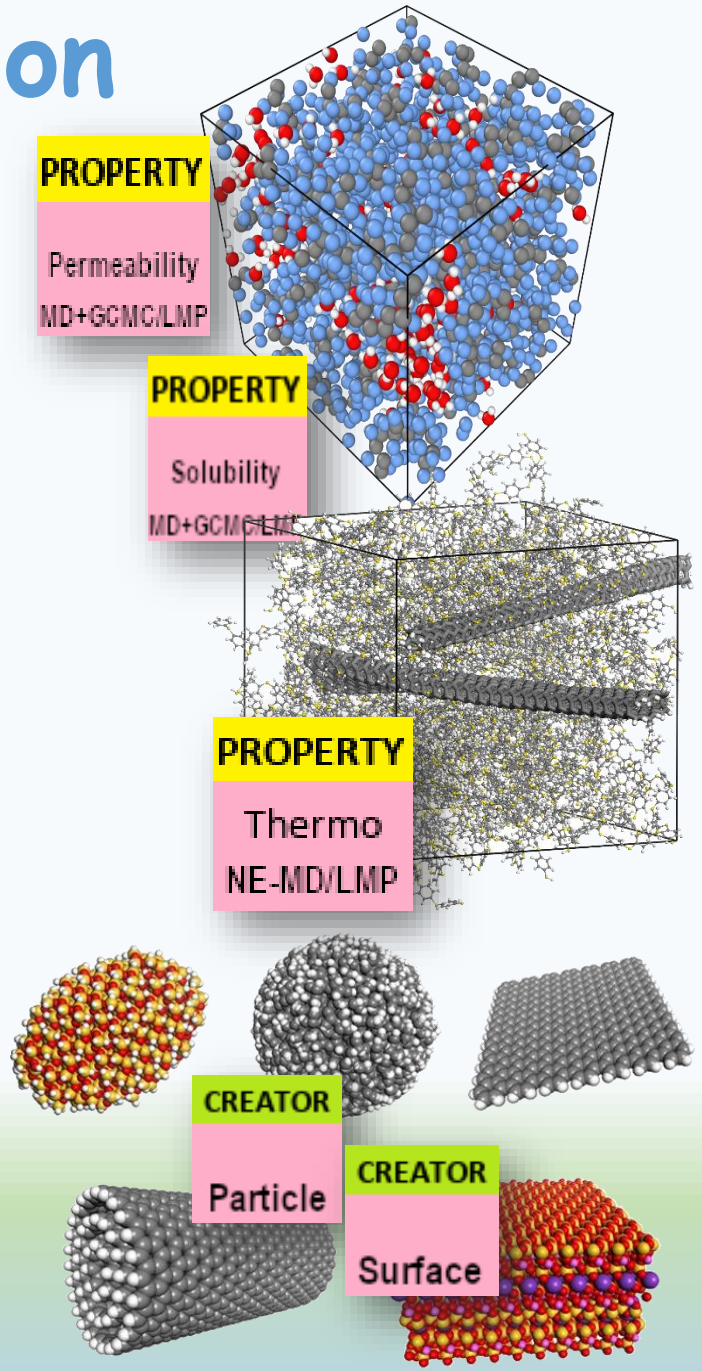
- structural
- mechanical
- thermophysical
- transport

M.A. Akhukov, V.A. Chorkov, A. A. Gavrilov, D.V. Guseva, P.G. Khalatur, A.R. Khokhlov, A.A. Kniznik, P.V. Komarov, M.V. Okun, B.V. Potapkin, V.Yu. Rudyak, D.B. Shirabaykin, A.S. Skomorokhov, S.V. Trepalin, **MULTICOMP package for multilevel simulation of polymer nanocomposites**, Computational Materials Science, V. 216, 2023, 111832, **https://doi.org/10.1016/j.commatsci.2022.111832**.

thank you for the attention

- ADDED PERMEABILITY, SOLUBILITY AND NE-MD THERMO MODULES
- ADDED SURFACE AND PARTICLE CONSTRUCTORS
- MODIFIED ATOM TYPING AND ADDED SUPPORT FOR AMBER FORCE FIELD
- MODIFIED VERSION OF THE DPD CONSTRUCTOR MODULE
- ADDED CALCULATION EXAMPLES:
  - Thermoconductivity calculation of the PPS / PPS+CNT composite
    (Knizhnik A. et al // Russian Supercomputing Days. – Cham : Springer Nature Switzerland, 2024. – C. 267-281)
  - PA clay strucute build
    (Akhukov M. A. et al. // Computational Materials Science. – 2023. – T. 216. – C. 111832.)
  - PE / PET /PTFE permeability and solubility calculation
    (Knizhnik A. et al. // Minerals. – 2023. – T. 13. – №. 9. – C. 1151.)
  - Thermoconductivity calculation of the aligned PE
- FIXED BUGS, EXTENDED DOCUMENTATION ETC…

MULTICOMP
multilevel simulation of polymer nanocomposites
RELEASE 1.2



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