Keldysh Institute of Applied Mathematics
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Computer Simulation of the Interaction of Metal Nanoparticles with a Substrate

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The work was supported by the Russian Science Foundation, project No. 21-71-20054

10th International Conference "Distributed Computing and Grid Technologies in Science and Education"
2023, July 3 – 7, Dubna, Russia

Goals and tasks

***Main goal** is a development of supercomputer technology for simulation of complex processes in technical micro- and nanosystems*

The technology includes the following components:

- *multi-scale mathematical models set;*
- *parallel numerical algorithms base;*
- *parallel software tools;*
- *applications in nanotechnologies.*

Achieved results:

A multi-level multi-scale approach to the calculations of actual problems of gas and plasma dynamics has been developed and tested.

2. Numerical methods for solving both independent and related problems that determine the behavior of the system at various scale levels.

3. Parallel algorithms and software packages for simulation of multi-scale problems.

4. A database on the properties of substances that includes: parameters of the gas medium, kinetic parameters of gases and metals, parameters for determining of boundary conditions.

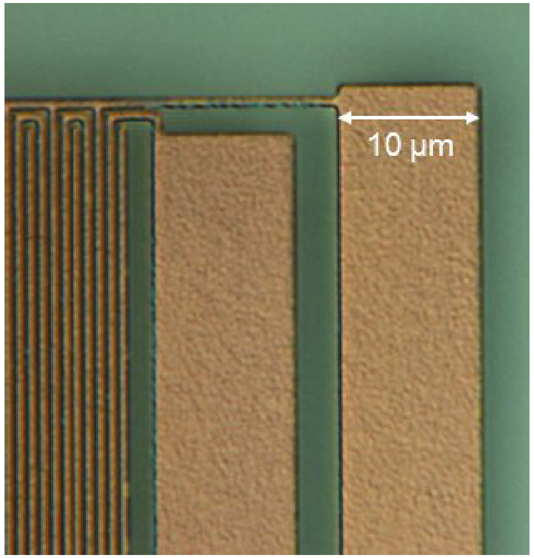
5. Model calculations for some actual nanotechnology problems.

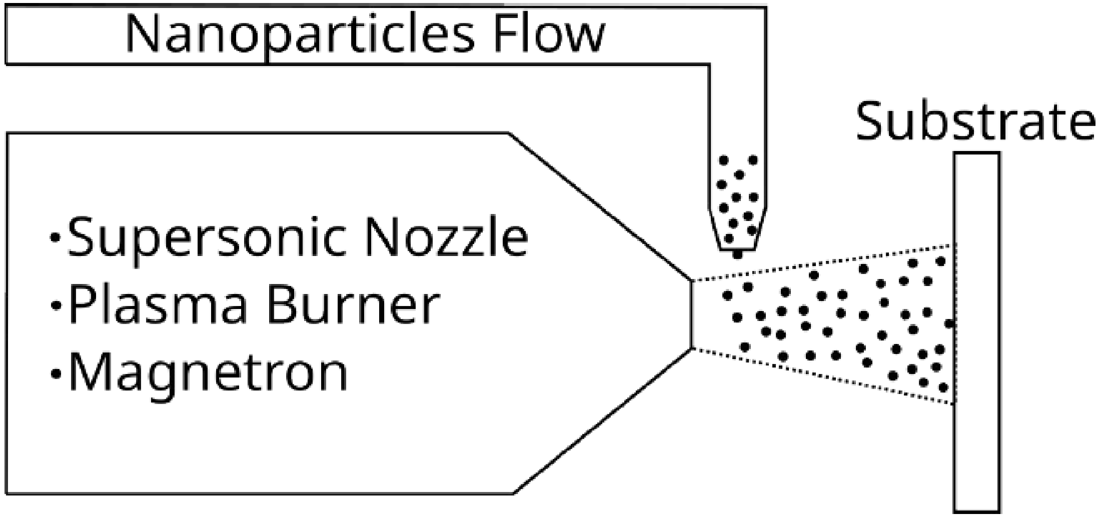
Metalic Nanoparticles Spraying

Application:
- protective coatings
- microelectronics
- medical equipment
- bio-sensors
etc.

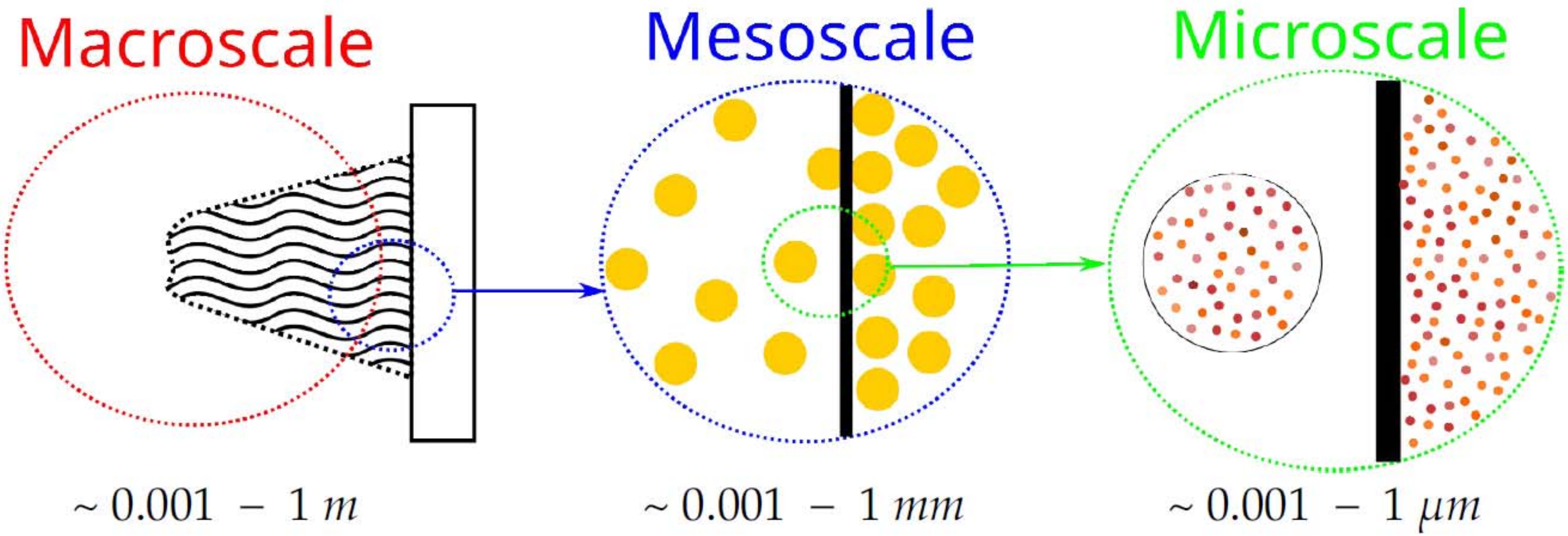
Technological methods:
- supersonic cold gasdynamics spraying
- plasma spraying
- magnetron spraying
etc.

Birkholz, M.; Ehwald, K.-E.; Wolansky, D.; Costina, I.; Baristiran-Kaynak, C.; Fröhlich, M.; Beyer, H.; Kapp, A.; Lisdat, F. (15 March 2010). “Corrosion-resistant metal layers from a CMOS process for bioelectronic applications”. *Surface and Coatings Technology*. **204** (12–13): 2055–2059.





Multiscale Analysis



Modeling approaches:
Macroscopic: Continuum Mechanics Models
Mesoscopic: Particle Methods
Microscopic: Molecular Dynamics
Macroscopic and Microscopic: CMM + MD
Macro-, Meso- and Microscopic: CMM + PM + MD

Mathematical Models and Numerical Methods

Mathematical models:

Macroscopic:
- Navier-Stocks equations
- Quasi Gas Dynamics equations
- Maxwell's electrodynamics

Mesoscopic:
- Large particles
- Smoothed particles
- Particle in cells
- Particle clouds

Microscopic:
- Classic Molecular Dynamics
- Quantum Molecular Dynamics
- Hartree-Fock approache
- Variational models

Numerical approaches:
- Splitting on physical processes
- Transitions between scales

Macroscopic:
- Cartesian grids
- Unstructured grids
- Hybrid block grids
- Finite Volume Method
- Explicit or Implicit Time schemes
- Spatial and Nonlinearity Iterations

Mesoscopic:
- Newton dynamics

Microscopic:
- Molecular dynamics equations
- Interaction potentials
- Spectral methods
- Grid methods
- Density functional method
- Method of atomic orbitals

Parallel technologies and Software tools

Parallel technologies:
- Domain decomposition
- Load balancing
- Hybrid computations

Parallel environments:
- MPI
- OpenMP
- CUDA
- Hybrids

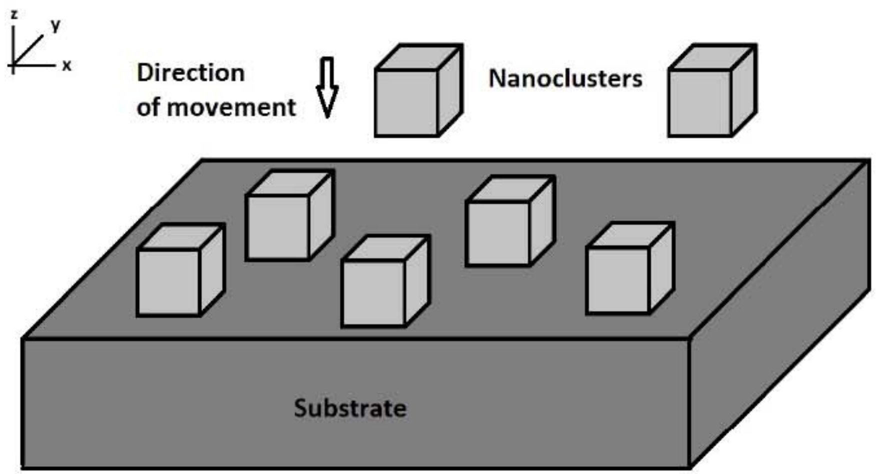
Programming languages:
- C/C++
- Fortran

Supercomputers:
- K100
- K10
- K60CPU
- K60GPU

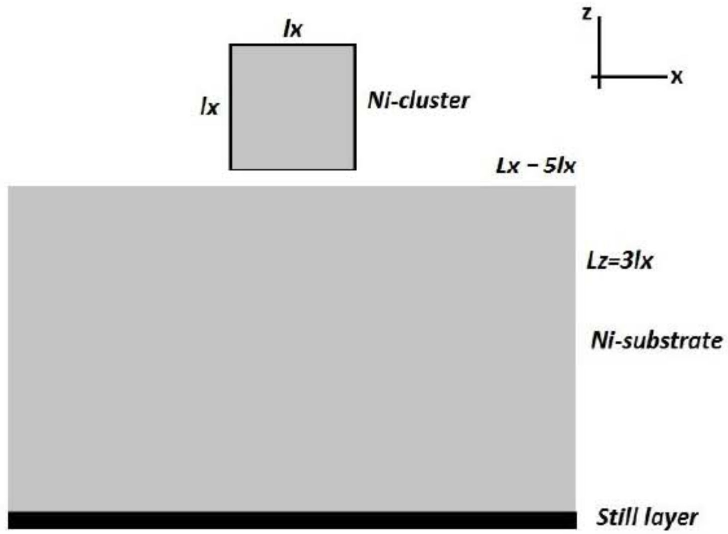
Self-maid software:
- GIMM_NANO tools:
  - GIMM_Main_GUI
  - GIMM_Mesh_Gen_Tool
  - GIMM_Visualizer
  - GIMM_Jobs_Management
  - GIMM_IO_Lib
  - GIMM_APP_MD_CPU_Gas_Metal
  - GIMM_APP_QGD_CPU
  - GIMM_APP_QGD_MD_CPU
  - GIMM_APP_QGD_MD_CPU
- Web-solutions:
  - KIAM_WMCS
  - KIAM_MDVIS
  - KIAM_MolSDAG_CPU
  - KIAM_MMD_WUI
  - KIAM_DIGITAL_TOOL_SERVER
  - KIAM_DIGITAL_TOOL_CLIENT

Mesoscopic solution

Problem formulation



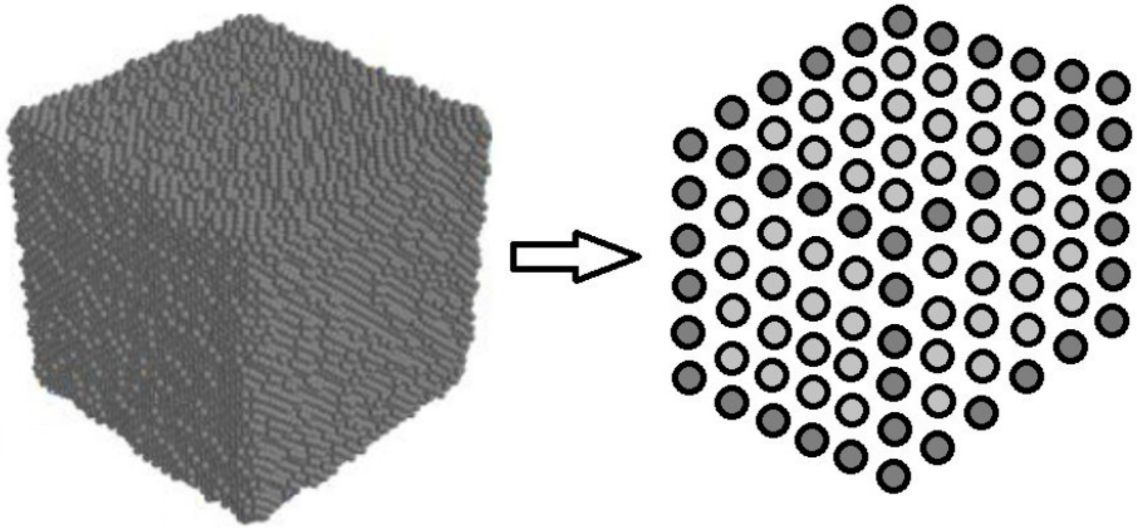
Model geometry of the problem



Computational Domain of preliminary numerical experiments

Nickel elementary cell on normal conditions:
a = 0.35314 nm
lx = 24*a = 8.475 nm

Mesoscopic Approach



Real nanocluster

Nanospheroid model

Nanospheroid model (form-function):

$$\delta(\boldsymbol{r}-\boldsymbol{r}_{\alpha,k}) \approx C_k(t)\cdot exp\left[-\left|\boldsymbol{r}-\boldsymbol{r}_{\alpha,k}\right|^2 / R_{\alpha,k}^2\right]$$

Neutral case (in electron units of mass and charge):

$$q_+ = +\left(\sqrt[3]{3N_a Z_a}\right)^2 \qquad q_- = -\left(\sqrt[3]{3N_a Z_a}\right)^2$$

$$m_+ = N_a m_a / m_e \qquad m_- = -\left(\sqrt[3]{3N_a Z_a}\right)^2$$

$\boldsymbol{r}_{\alpha,k}$	–	radius vector of k-spheroid of α sort
$\alpha = -, +$	–	nanospheroid sort
$C_k(t)$	–	normalization parameter
$R_{\alpha,k}$	–	effective radius
$q_{\alpha,k} \equiv q_\alpha$	–	charge of particle of α sort
$m_{\alpha,k} \equiv m_\alpha$	–	mass of particle of α sort
N_a, m_a, m_e	–	number and mass of ions, mass of electrons

Electromagnetics Field Equations

Maxwell equations:

$$divB = 0 \qquad div(\varepsilon_a E) = \rho$$

$$\frac{\partial B}{\partial t} = -\,rotE \qquad \frac{\partial}{\partial t}(\varepsilon_a E) = rot\left(\frac{1}{\mu_a}B\right) - j$$

Electric field as sum of wave processes and particles evolution:

$$E = E^{(w)} + E^{(p)} \qquad E^{(p)} = -\,\nabla\varphi$$

$$div\left(\varepsilon_a E^{(w)}\right) = 0 \qquad div(\varepsilon_a \nabla\varphi) = -\,\rho$$

$$\frac{\partial}{\partial t}\left(\varepsilon_a E^{(w)}\right) = rot\left(\frac{1}{\mu_a}B\right) - j - \frac{\partial}{\partial t}\left(\varepsilon_a E^{(p)}\right)$$

div, rot	–	divergence and rotor
B	–	magnetic induction vector
ε_a	–	absolute dielectric permeability of the medium
E	–	electric field strength vector
$\rho = \rho_e + \rho_i$	–	volume charge density divided into positive and negative comp.
μ_a	–	absolute magnetic permeability of the medium
j	–	current density vector (generated by particles)
$E^{(w)}$	–	wave processes part of electric field strength
$E^{(p)}$	–	particles evolution part of field strength
φ	–	quasi-static potential of electromagnetic field

Nanocluster Evolution Equations

Newton dynamic with the Lorentz force:

$$\frac{d\boldsymbol{r}_{\alpha,k}}{dt} = \boldsymbol{v}_{\alpha,k} \qquad \frac{d\boldsymbol{p}_{\alpha,k}}{dt} = q_{\alpha,k}\left(\boldsymbol{E} + \left[v_{\alpha,k} \times \boldsymbol{B}\right]\right)$$

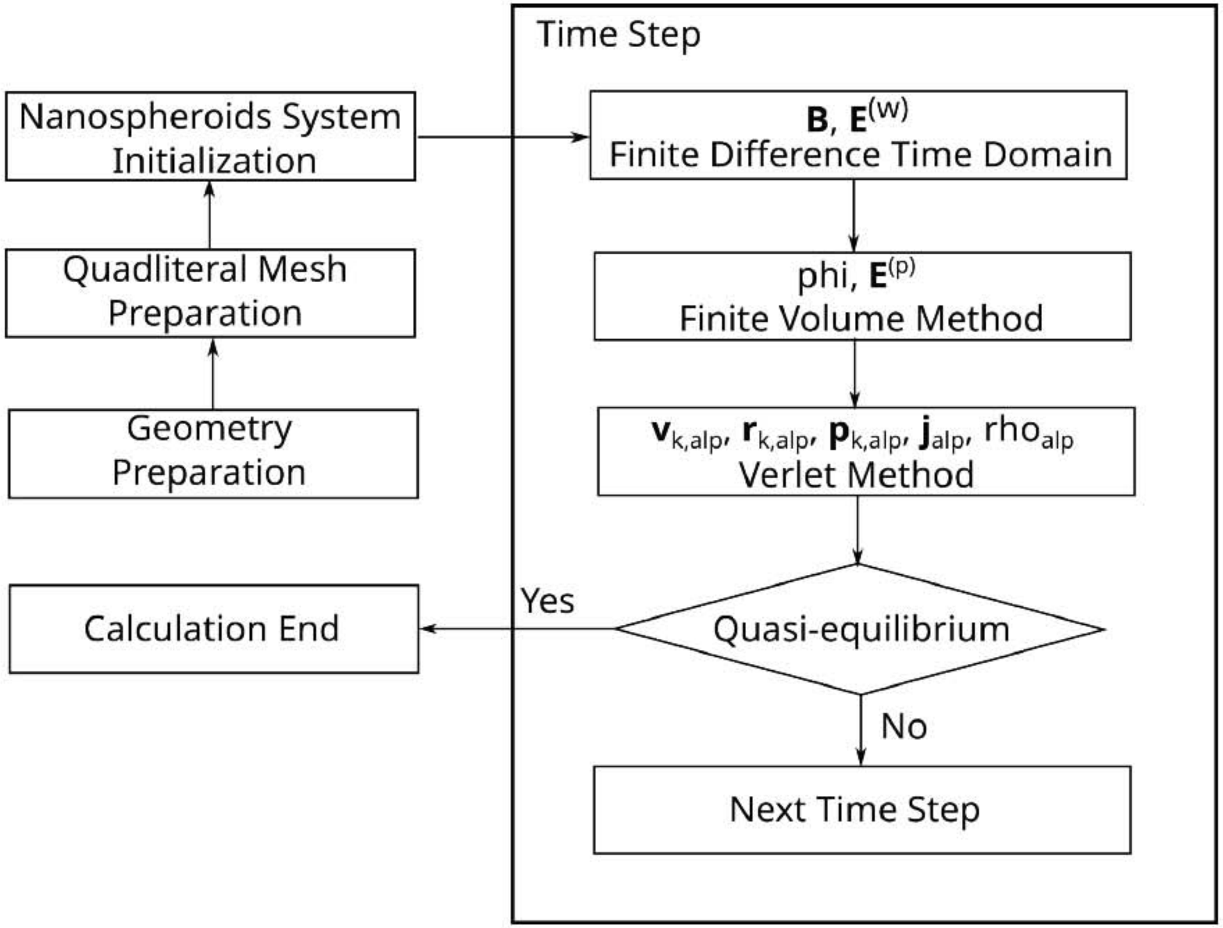
$$\boldsymbol{p}_{\alpha,k} = m_{\alpha,k}\boldsymbol{v}_{\alpha,k}$$

$$\rho_\alpha = \sum_{k=1}^{N_\alpha} \boldsymbol{q}_{\alpha,k}\delta\left(\boldsymbol{r} - \boldsymbol{r}_{\alpha,k}\right)$$

$$\boldsymbol{j}_\alpha = \sum_{k=1}^{N_\alpha} \boldsymbol{q}_{\alpha,k}\delta\left(\boldsymbol{r} - \boldsymbol{r}_{\alpha,k}\right)\boldsymbol{v}_{\alpha,k}$$

$\boldsymbol{r}_{\alpha,k}$	–	radius vector of k-spheroid of α sort
t	–	time
$v_{\alpha,k}$	–	velocity vector of k-spheroid of α sort
$\boldsymbol{p}_{\alpha,k}$	–	momentum vector of k-spheroid of α sort
$\alpha = -, +$	–	nanospheroid sort
$k = 1,\ldots,N_a$	–	index of nanospheroid of α sort
$m_{\alpha,k} = m_\alpha$	–	mass of nanospheroid of α sort
$q_{\alpha,k} = q_\alpha$	–	charge of nanospheroid of α sort
N_a	–	number of nanospheroids of α sort

Numerical Algorithm



boundary conditions

$\boldsymbol{E}$, $\boldsymbol{B}$ - inlet TE-wave, absorbing

$\boldsymbol{r}_{\alpha,k}$, $\boldsymbol{v}_{\alpha,k}$ - free-out, adhesion or absorption

Initial Conditions

$$\boldsymbol{E}^{(w)} = 0$$

$$\boldsymbol{B} = 0$$

$$\boldsymbol{E}^{(p)} = \boldsymbol{E}_0(x,y,z)$$

$$\boldsymbol{r}_{\alpha,k} = \boldsymbol{r}_{0,\alpha,k}$$

$$\boldsymbol{v}_{\alpha,k} = \boldsymbol{v}_{Maxwell,\alpha,k}$$

Numerical methods and parallel solution

1. **Unstructured grids**
2. **Finite Difference Time Difference scheme for Maxwell equations**
3. **Domain decompositon for cluster nodes**
4. **Sub-domain decomposition for CPU threads**

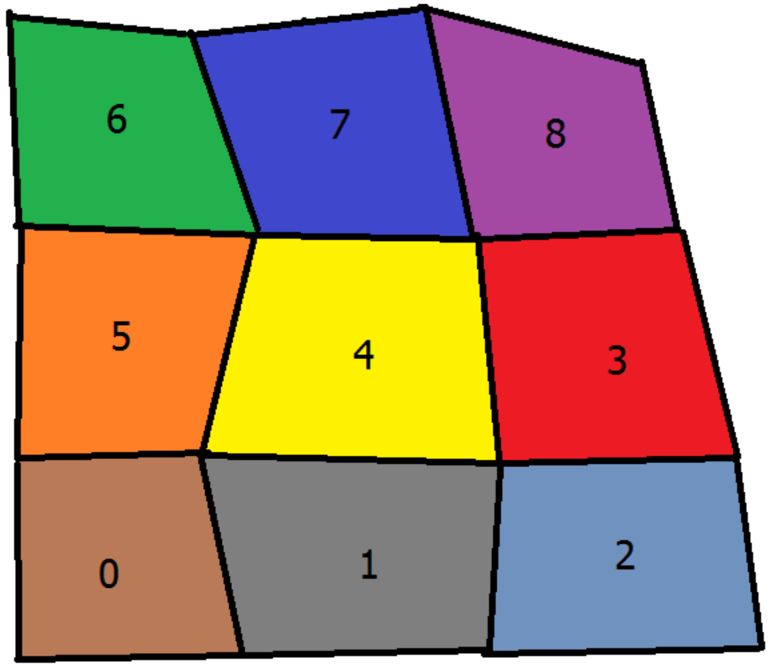
Domain decomposition

The Peano's curves technique (MPI-processes)

$$p = p_1 p_2 p_3$$

$$\frac{p_1}{p_2} \approx \frac{N_1}{N_2} \qquad \frac{p_1}{p_3} \approx \frac{N_1}{N_3} \qquad \frac{p_2}{p_3} \approx \frac{N_2}{N_3}$$

p	–	total number of threads
p_1, p_2, p_3	–	threads per direction (x,y,z)
N_1, N_2, N_3	–	number of mesh elements per direction (x,y,z)



Parallel realization for particles

1. **Conservative Adams Scheme for Newton's equations**
2. **Domain decompositon for cluster nodes**
3. **Local load-balancing algorithm into each cluster node**
4. **Global load-balancing algoritm between cluster nodes**

Load balancing algorithm:

1) Initial uniform splitting and calculation by *p*-threads

2) Determining the time $t_k \ (k = 0,\dots,p-1)$ of k-thread computing

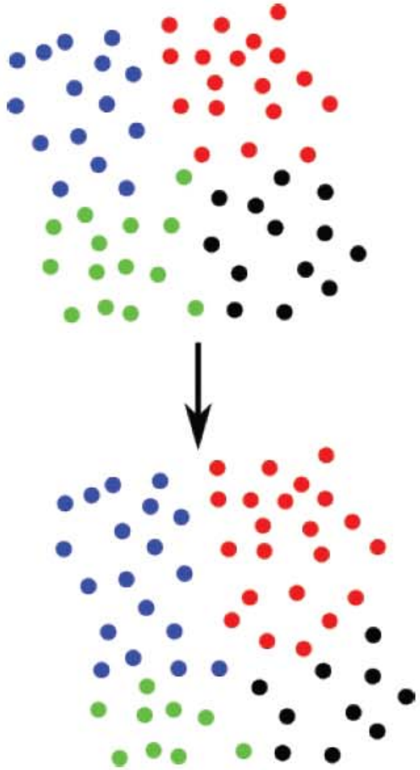
3) Calculation of the average execution time and relative times dispersion:

$$t_s = \frac{1}{p}\sum_{k=0}^{p-1} t_k, \quad \sigma = \max_k \left|(t_k - t_s)/t_s\right| \cdot 100\%$$

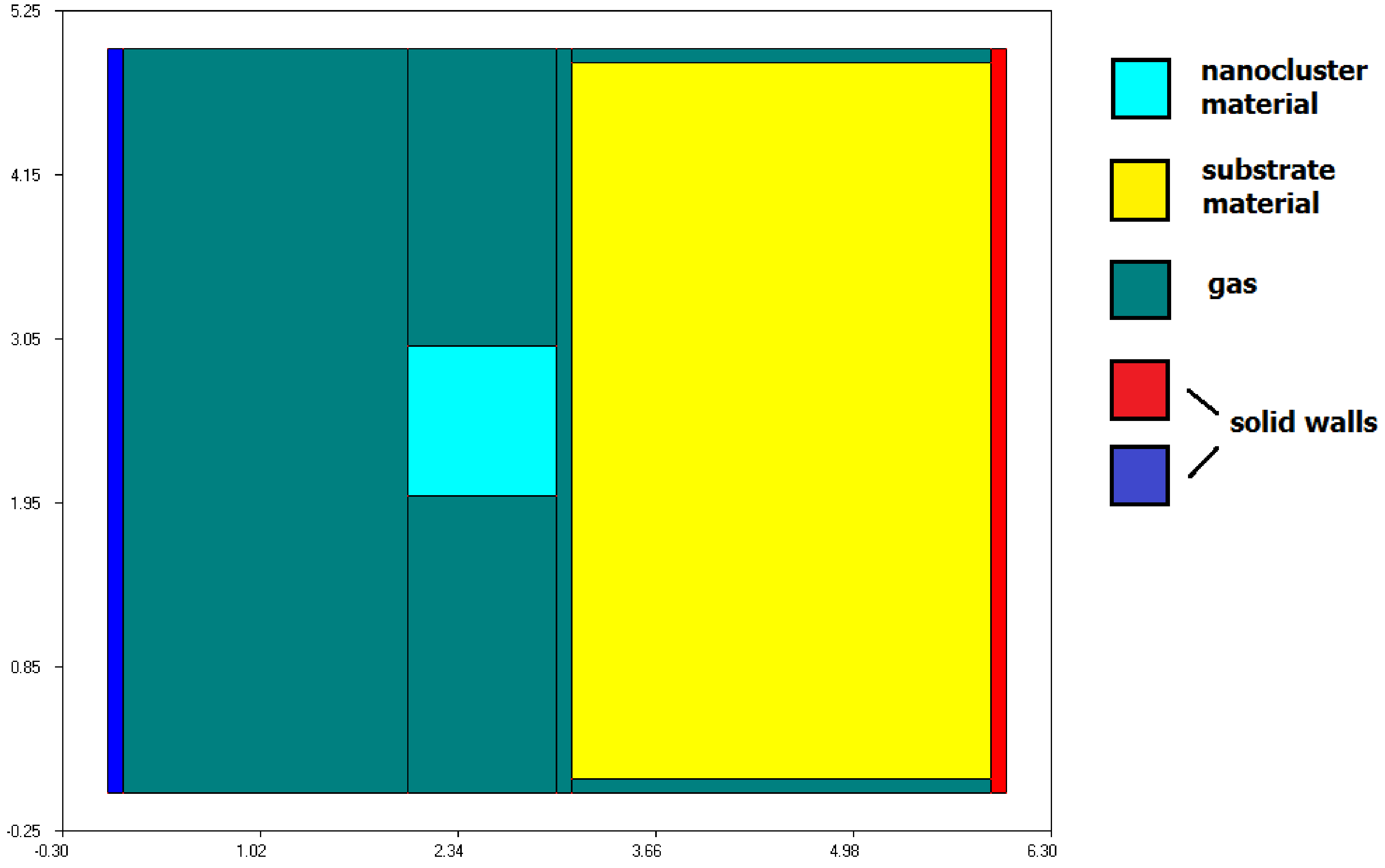
4) If $\sigma > 5\%$ redistribution of nanospheroids by threads:

$$N_k = N_k + \gamma N \cdot \frac{q_k}{Q}, \quad q_k = \frac{N_k}{t_k}, \ k = 0,\dots,p-2$$

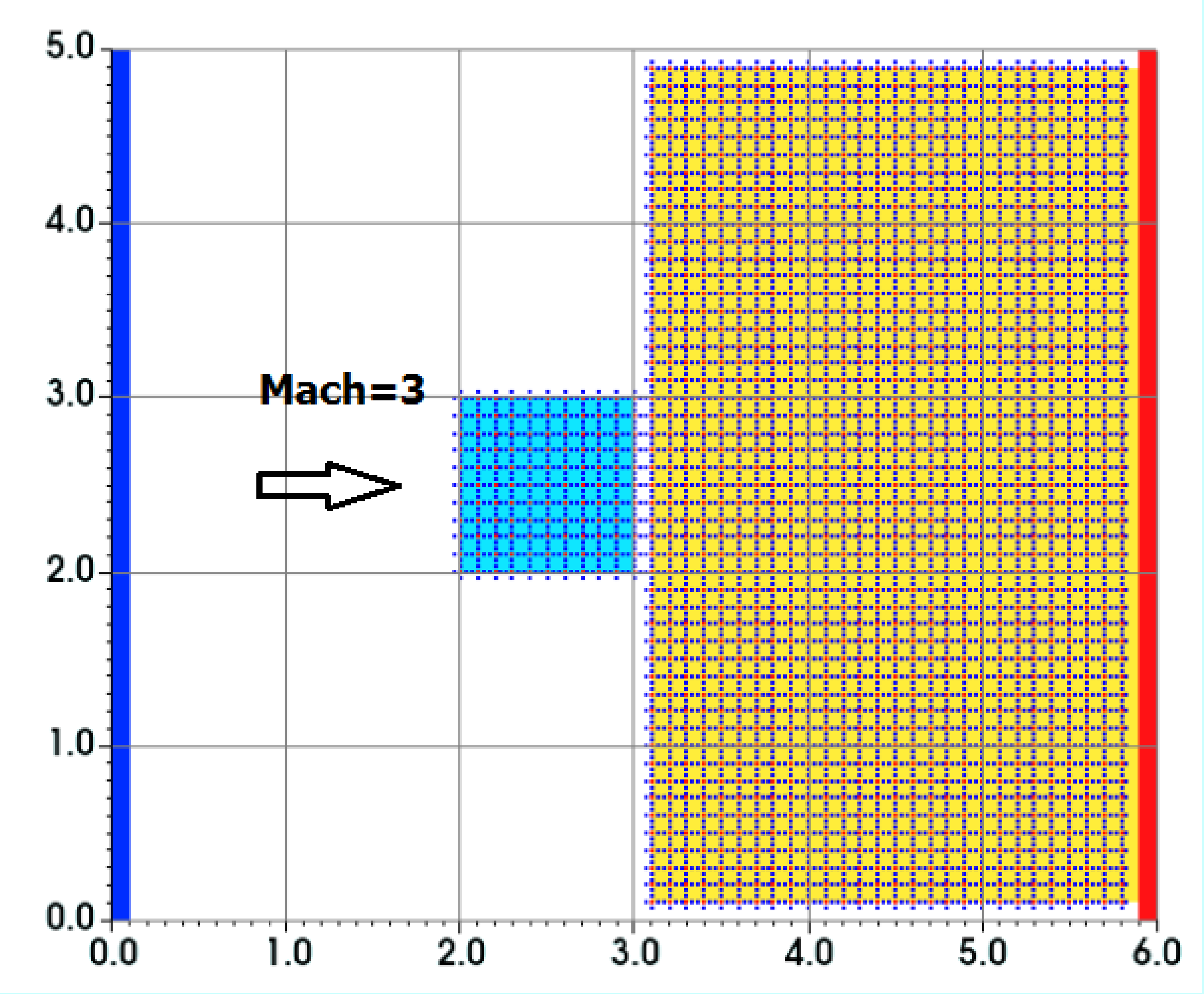
$$N_{p-1} = N - \sum_{k=0}^{p-2} N_k, \ N = N_+ + N_-, \quad Q = \sum_{k=0}^{p-2} q_k, \ \gamma \sim 0.05$$



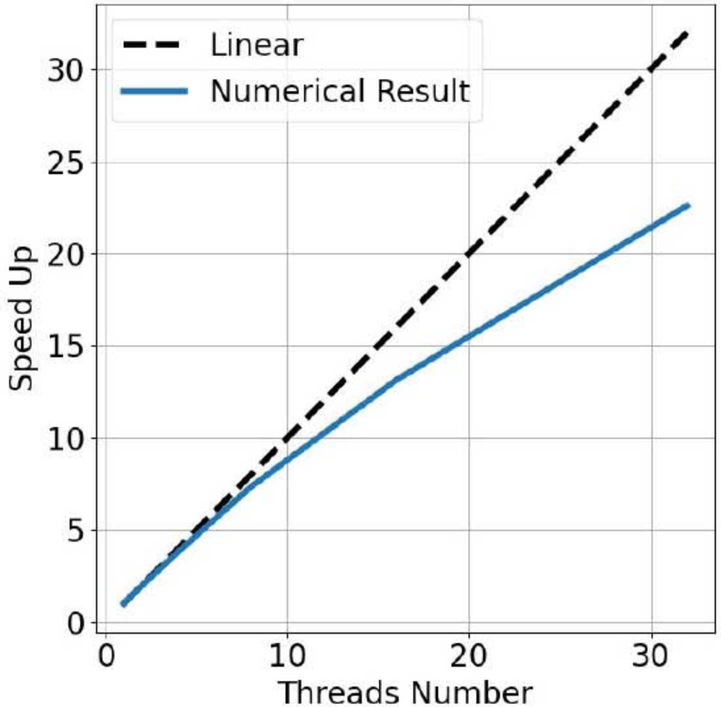
Interaction of the nanocluster with the substrate

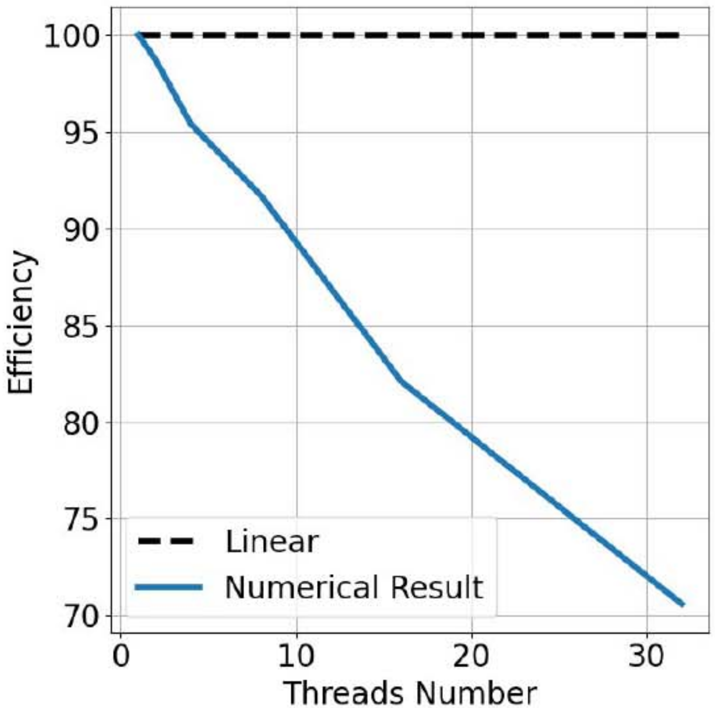


Initial particles distribution



Speed UP and Efficiency for one cluster node

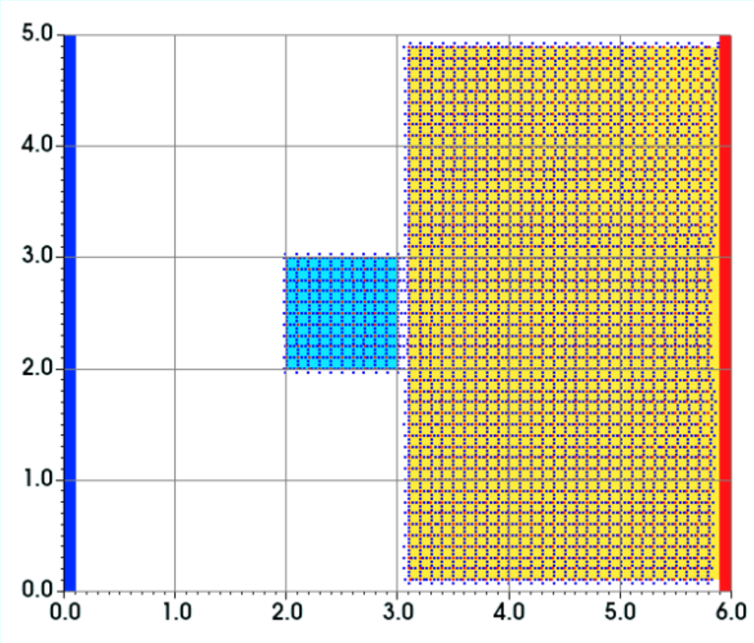




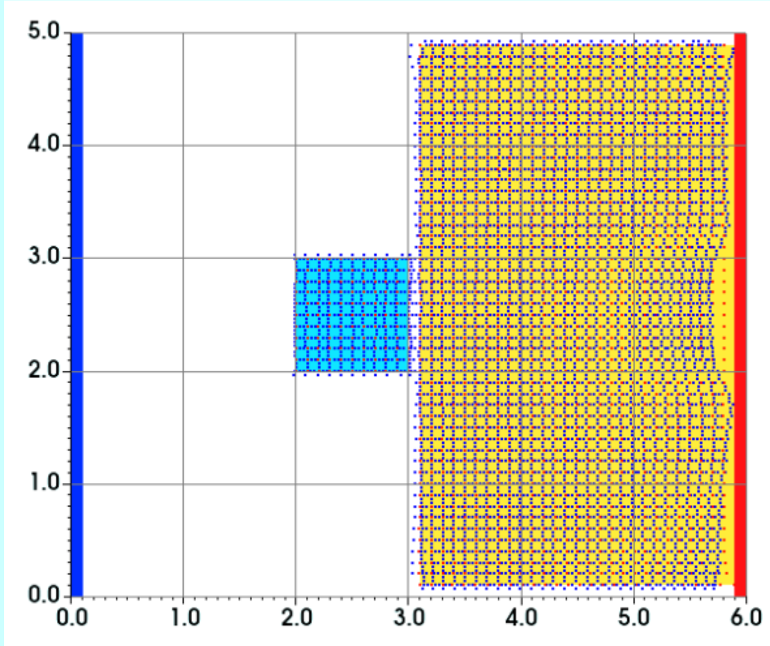
Node of K60 GPU:
2 x Intel Xeon Gold 6142 v4, 16 threads
Task: quasi-equilibrium (20000 time steps) of 25386 nanospheroids

Simulation results

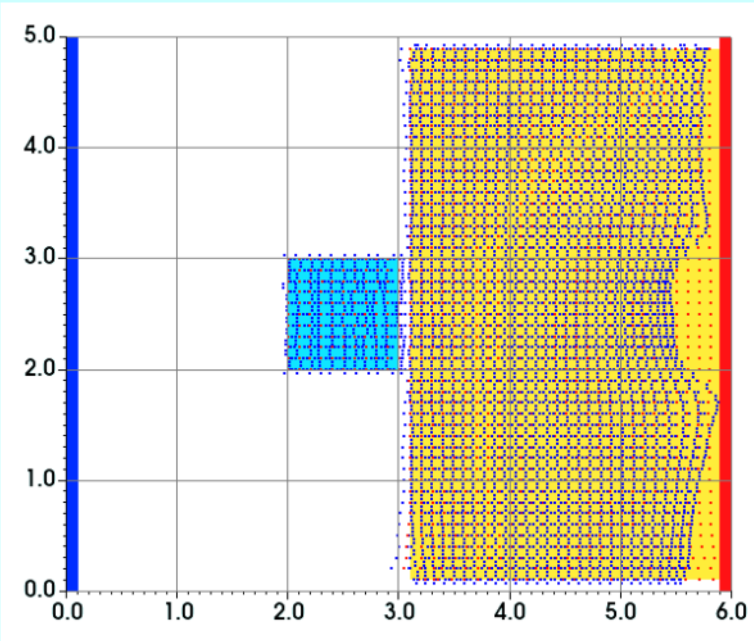
1 ns



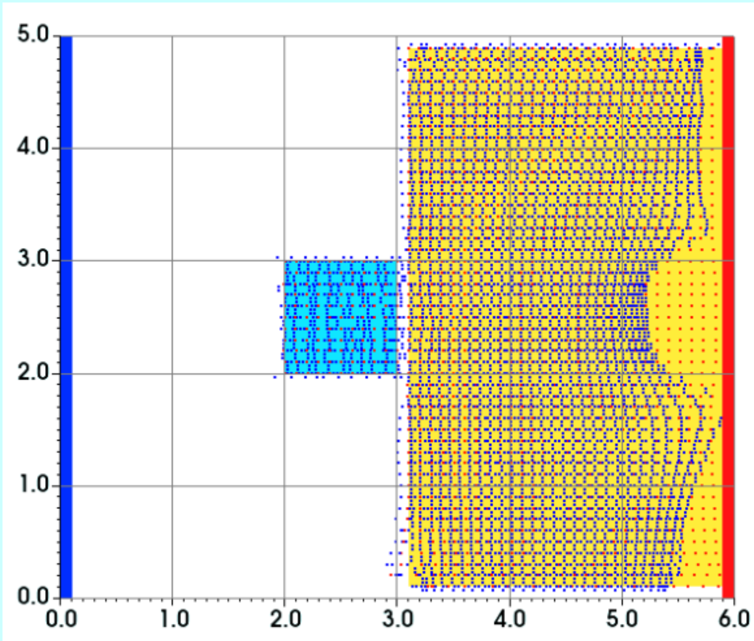
2 ns



3 ns



4 ns



Conclusion

- The complex technology of supercomputer modeling of problems of deposition of metal nanoparticles on substrates is presented.
- A mesoscopic approach to solving spraying problems is considered.
- A sputtering model combining macroscopic and microscopic levels based on Maxwell's equations and equations of particle dynamics is proposed.
- Numerical methods have been developed that combine the grid method FDTD and particle methods PIC and SPE.
- Parallel algorithms for implementing numerical schemes based on MPI and OpenMP technologies have been created.
- Model calculations were carried out that demonstrated the operability and adequacy of the developed computing technology.

Thank you for the attention!