**Keldysh Institute of Applied Mathematics
Russian Academy of Sciences**

Parallel algorithms for calculating problems of supersonic cold gas-dynamic spraying nanoparticles on substrates

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Goals and tasks

Main goal is a development of supercomputer technology for modeling the complex processes in technical micro- and nanosystems
Specific goal is a application of the technology to solution of particular problem

The technology includes the following components:
 - multiscale mathematical models set;
 - parallel numerical algorithms base;
 - parallel software tools;
 - applications in nanotechnologies.

Achieved results:
1. A multilevel multiscale 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 modeling multiscale problems.
4. A database on the properties of substances that includes:
     macroparameters of the gas medium (pure gases and mixture) and metals,
     parameters for determining the 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.

10 µm

Nanoparticles Flow

Substrate

- Supersonic Nozzle
- Plasma Burner
- Magnetron
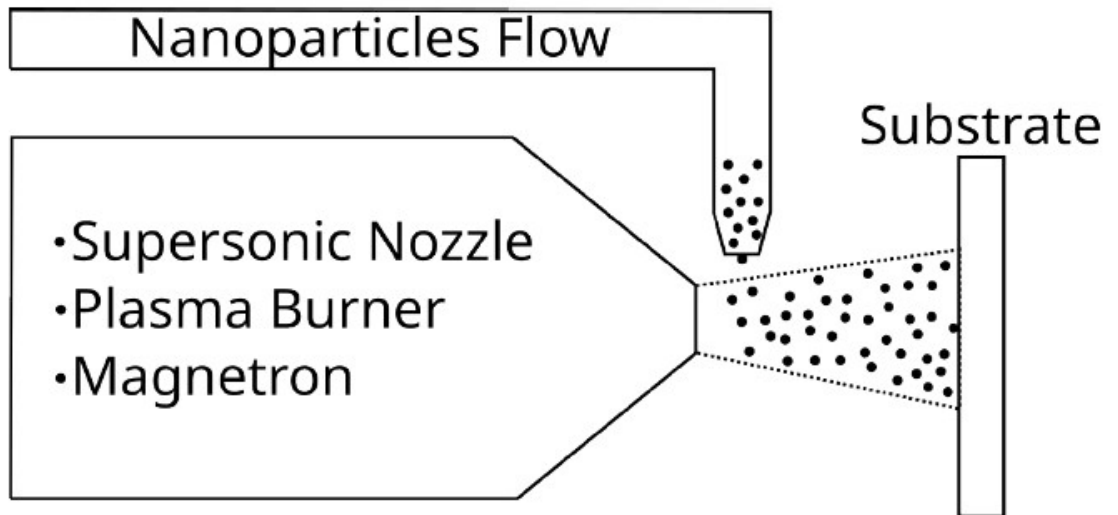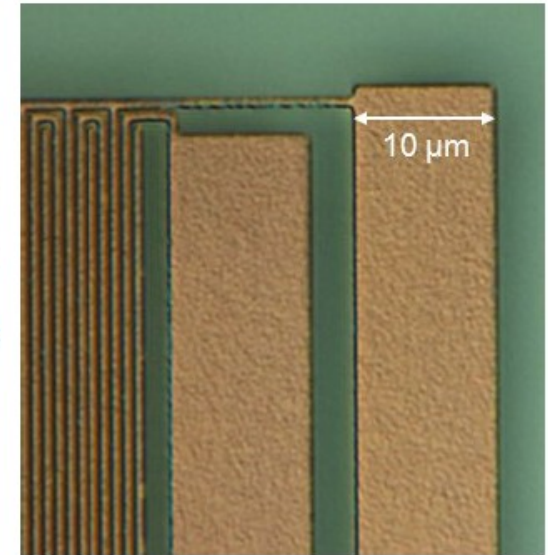
Multiscale Analysis
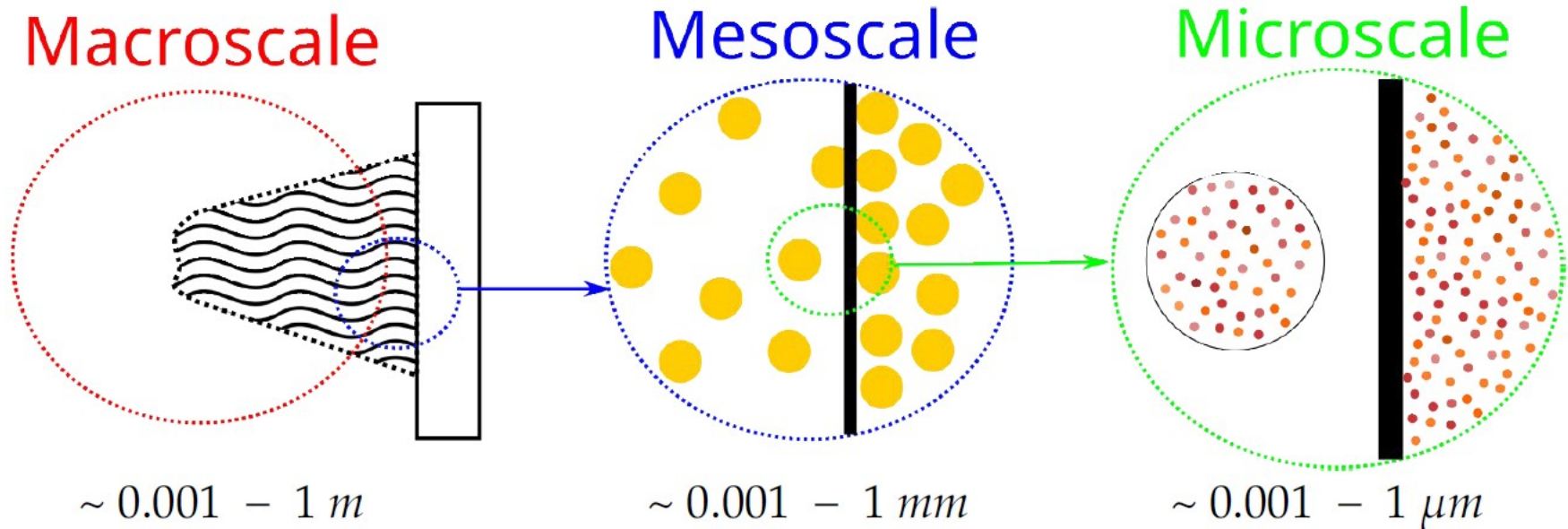
Modeling approaches:
Macroscopic: Continuum Mechanics Models
Mesoscopic: Particle Methods
Microscopic: Molecular Dynamics
Macroscopic and Microscopic: CMM + MD
Macro-, Meso- and Microscopic: CMM + PM + MD

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 approach
   Variational models

Numerical approaches:
   Splitting by 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
   Spectral methods
   Grid methods
   Density functional theory
   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 – 86 nodes, 82 TFlops
  K60GPU
  K120
* http://ckp.kiam.ru

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**
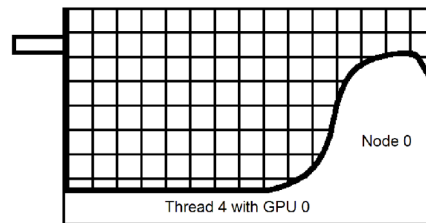   **KIAM_DIGITAL_TOOL_CLIENT**

Parallel realization

- **The main method of parallelization - partition into domains of equal power.**
- **Each domain is divided into "boxes of interaction".**
- **Topology distribution on domains and boxes - a three-dimensional lattice.**
- **Topology exchanges - a three-dimensional torus.**
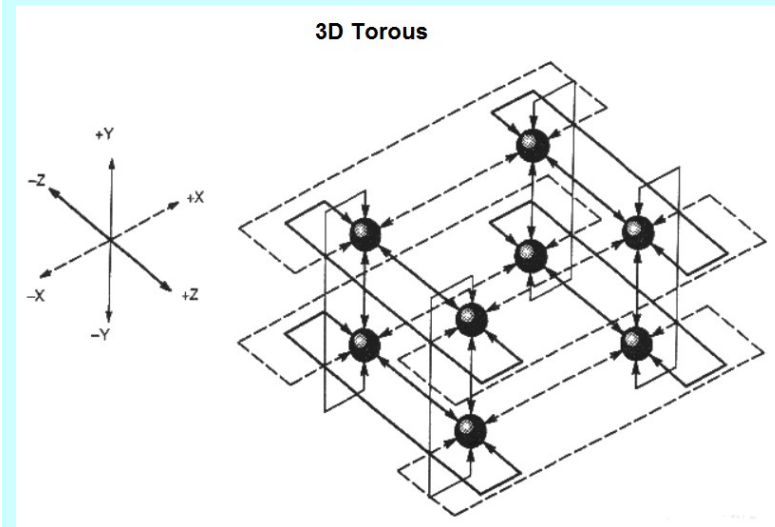- **Realization – MPI + OpenMP**

QGD+NPD/MD domain decompositions

Node 3	Node 4	Node 5
Node 0	Node 1	Node 2

Node 0

Thread 0 | Thread 1 | Thread 2 | Thread 3
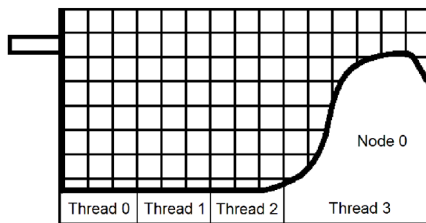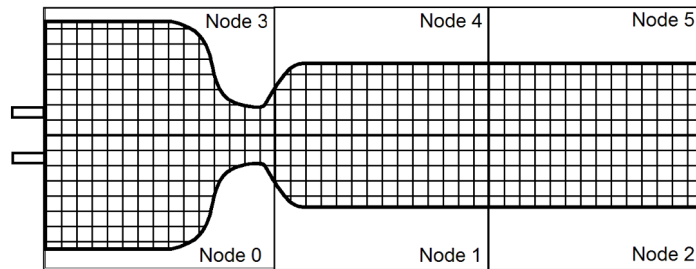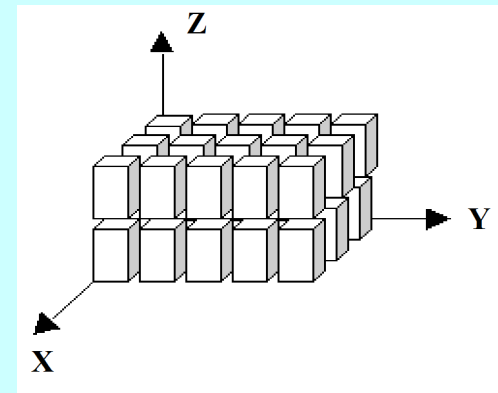
Quasi Gas Dynamic Computations

Node 0

Thread 4 with GPU 0

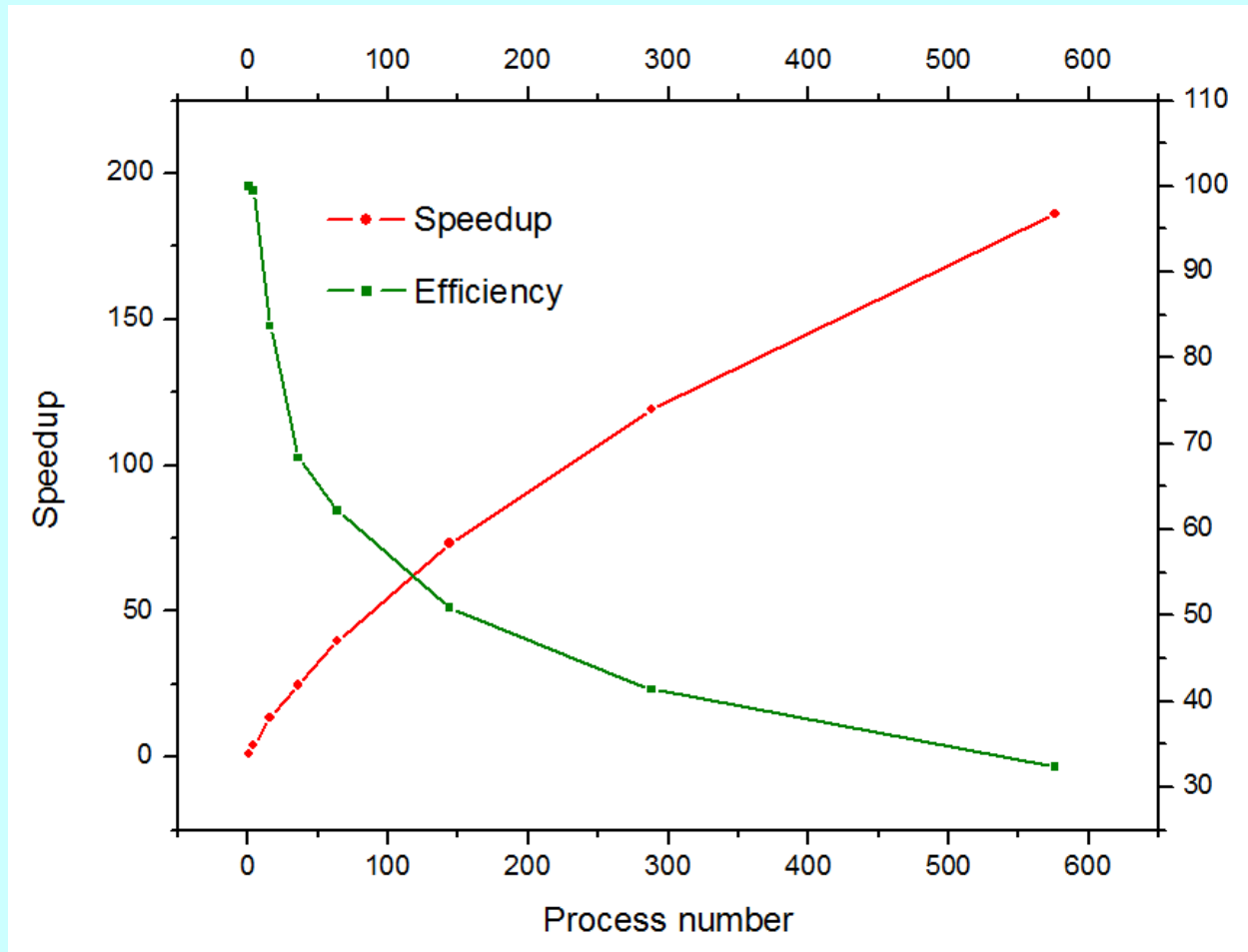Molecular Dynamic Computations

3D Torous

Test for speedup and efficiency

MPI+OpenMP solution
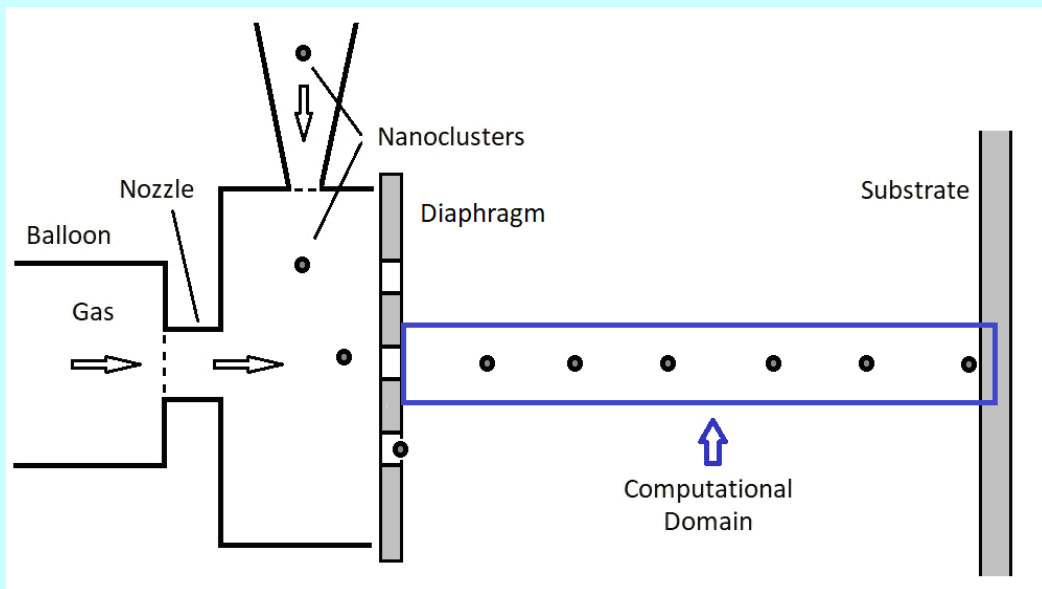**Macroscopic level: 2400000 cells of 3D Grid**
Microscopic level: 2825358 particles in gas and nanoparticles
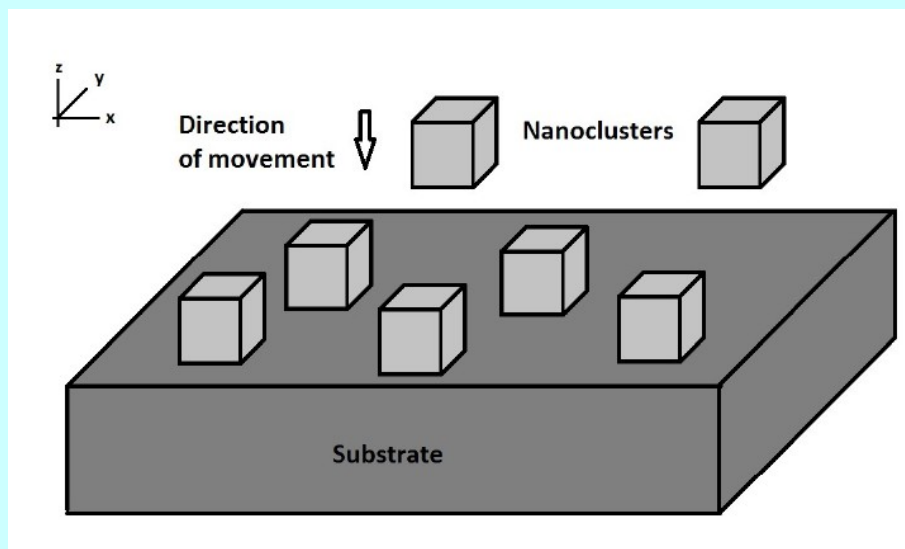**250000 computation steps**

Supersonic Cold Gas-Dynamic Spraying Nickel Nanoclusters on Substrate
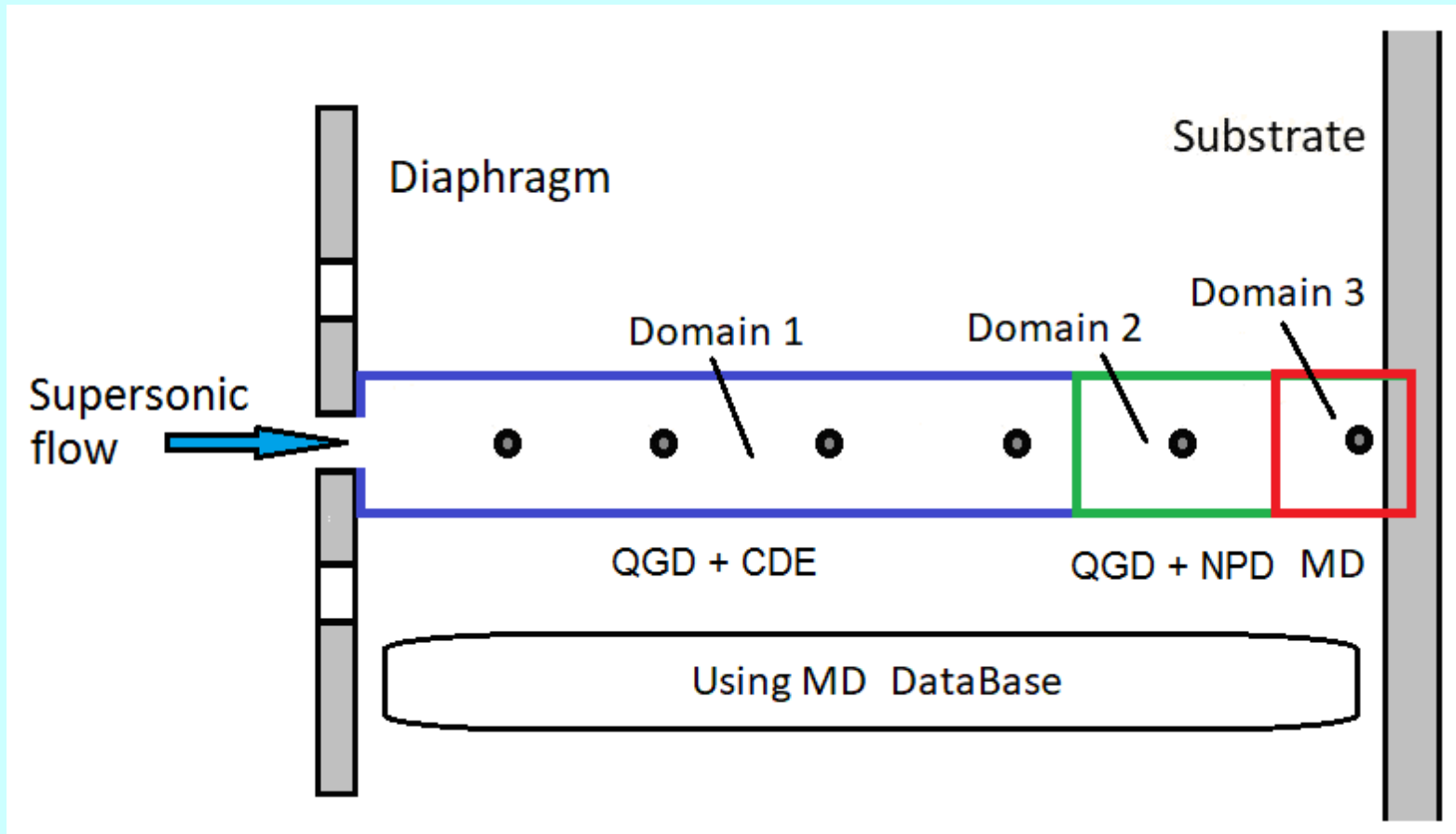

Technology process
Computational domain

Zoom of substrate zone

Multiscale approach

Macroscopic model – Quasi-gas-dynamics equations (QGD)
                                        + convection-diffusion equations (CDE)
Mesoscopic model – QGD + Newton's particle dynamics (NPD)
Microscopic model – Molecular dynamics (MD)

Macroscopic basic equations

On the macroscopic level, the quasi-gasdynamic system of equations one component gas is written in the form, that invariant with respect to the coordinate system. In dimensional variables in SI units, this system together with the equations of state and constraints will be written as follows:

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \mathbf{W}^{(\rho)} = 0; \quad \frac{\partial (\rho u_k)}{\partial t} + \operatorname{div} \mathbf{W}^{(\rho u_k)} = 0, \ k = x, y, z; \quad \frac{\partial E}{\partial t} + \operatorname{div} \mathbf{W}^{(E)} = 0;$$

$$E = \frac{1}{2}\rho |\mathbf{u}|^2 + \rho\varepsilon, \ \varepsilon = c_V T, \ H = \frac{E+p}{\rho}, \ p = Z\rho\Re T, \ \gamma = \frac{c_p}{c_V}, \Pr = \frac{\mu c_p}{\chi}, \operatorname{Ma} = \frac{|\mathbf{u}|}{a}, \operatorname{Re} = \frac{\rho |\mathbf{u}| \lambda}{\mu};$$

(1)

$$\frac{\partial C}{\partial t} + \operatorname{div} \mathbf{W}^{(C)} = 0.$$

(2)

It is assumed here that the gas is characterized by mass and number density $\rho = \rho_g = m_g n$ and $n = n_g$ (m_g is the molecule's mass), temperature $T = T_g$ and macroscopic velocity $\mathbf{u} = \mathbf{u}_g$. Other parameters of the gas are as follows: $p = p_g$ are the partial pressures of gas; $E = E_g$, H_g and ε_g are the densities of total energy, enthalpies and internal energies; $\mu = \mu(T_g)$, $D = D(T_g)$, $\chi = \chi(T_g)$ are the kinetic coefficients of gas, namely: coefficients of dynamic viscosity, diffusion and thermal conductivity. Variables $Z = Z(T_g, \rho_g)$, $\gamma = \gamma(T_g, \rho_g)$, $c_V = c_V(T_g)$, $c_p = c_p(T_g)$ and $\Re = k_B / m_g$ are the compressibility coefficients, adiabatic exponents, specific heat capacities and individual gas constants (k_B is the Boltzmann constant); $\Pr$, Ma and Re are the Prandtl, Mach and Reynolds numbers; $a = a_g$ is the sound speed, $\lambda = \lambda_g$ is the average free path length; C is the macroscopic concentration of nanoclusters; vectors $\mathbf{W}^{(\rho)}$, $\mathbf{W}^{(\rho u_k)}$, $\mathbf{W}^{(E)}$ coincide with the fluxes of density, corresponding components of the momentum density and energy density up to sign, vector $\mathbf{W}^{(C)}$ is the flux that describes of convection-diffusion process of nanoclusters.

Meso- and microscopicc equations

On the mesoscopic level we use the Newton's equations

$$M_k \frac{d\mathbf{V}_k}{dt} = \mathbf{F}_k, \quad \mathbf{V}_k = \frac{d\mathbf{R}_k}{dt}, \quad k = 1, ..., N_p. \tag{3}$$

Here $M_k, \mathbf{V}_k, \mathbf{R}_k$ are mass, velocity vector, radius vector of nanoclusters, $\mathbf{F}_k$ is summarized force that acts on the k-th nanocluster, N_p is the number of nanoclusters.

On the microscopic level, the molecular dynamics method was used for modeling. In the case of the study of particles of 2 types (metal and gas), the system of equations looks like this

$$m_l \frac{d\mathbf{v}_{l,i}}{dt} = \mathbf{F}_{l,i}, \quad \frac{d\mathbf{r}_{l,i}}{dt} = \mathbf{v}_{l,i}, \quad i = 1, ..., N_l, \quad l = g, m, \tag{4}$$

where i is the particle number, l is the particle kind (g means the molecules of gas, m means the atoms of metal in the nanocluster), N_l is the total number of particles of kind l, m_l is the mass of particle of kind l, $\mathbf{r}_{l,i}$ and $\mathbf{v}_{l,i}$ are the position and the velocity vectors of the i-th particle of kind l, $\mathbf{F}_{l,i}$ is the resultant force acting on the i-th particle. The forces depend on the interaction potentials. In this work, the Lennard-Jones potential is used for the gas-metal interaction, the potential of Mi "n-6" is used for the gas-gas interaction, and the embedded atom model is used for the metal-metal interaction.

The systems of equations (1)-(4) are closed by the initial and boundary conditions. The initial conditions for both systems are taken in accordance with the equilibrium state of the gaseous medium in the absence of interaction with external factors. Boundary conditions for QGD equations on the free surfaces of the computational domain are the so-called "soft" ones. A constant flow is set at the inlet to the medium with parameters determined by the nozzle configuration and cylinder pressure. Boundary conditions for MD equations are required only for the lateral surfaces of the computational domain, where periodic boundary conditions are used.

Block diagram of the general calculation algorithm
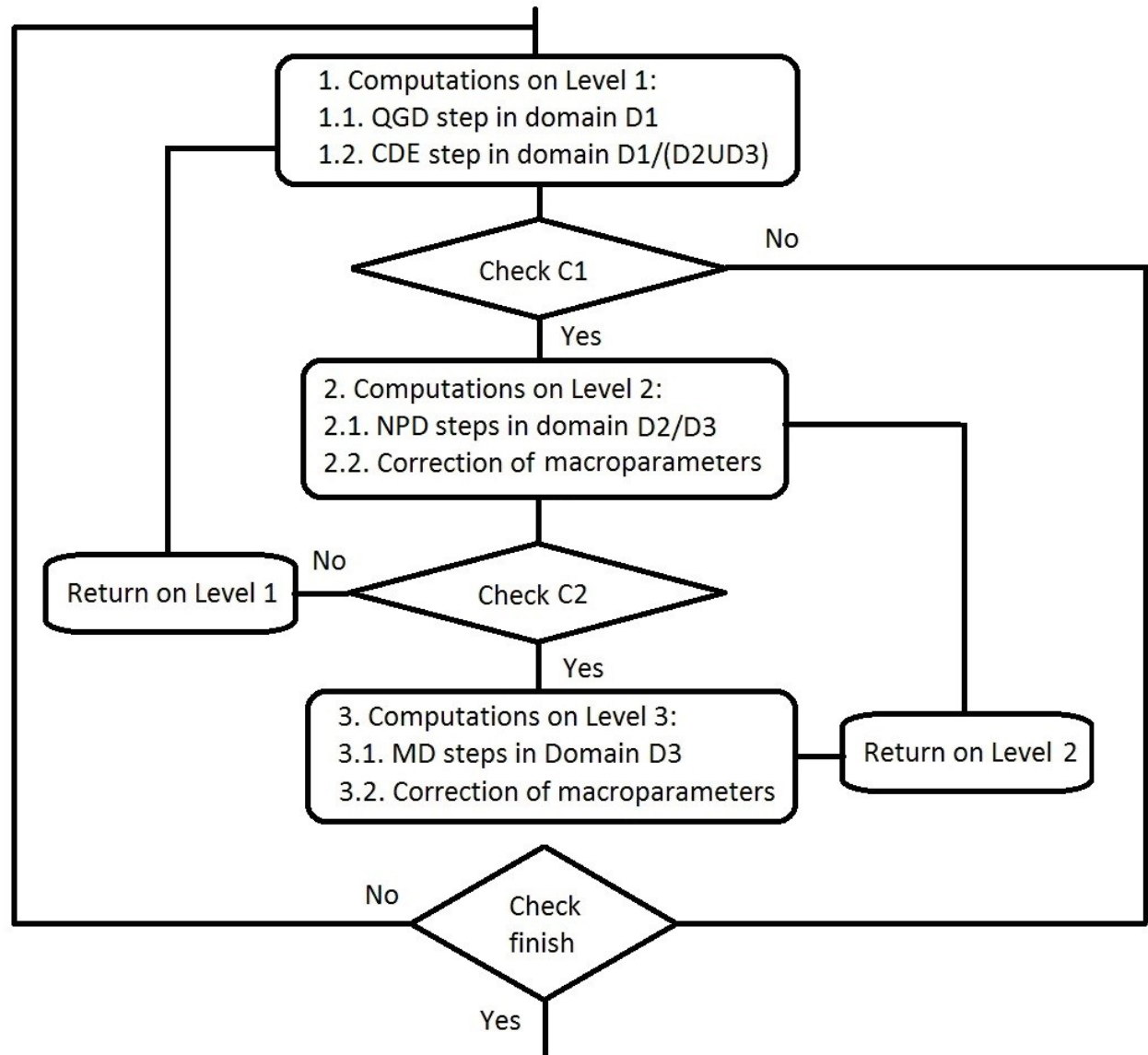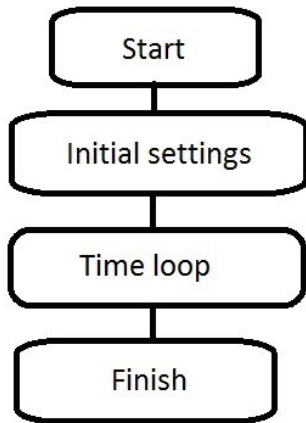
Model geometry
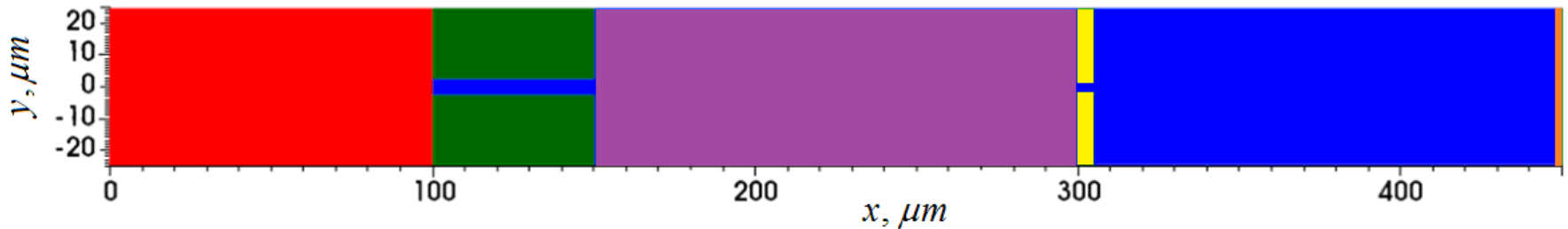
Design geometry includes a balloon (red), a nozzle (green), a nanocluster filling zone (violet), a diaphragm (yellow), a nanocluster transportation zone (blue) and a substrate (orange)

The goals of numerical modeling:
- analysis of spraying process
- optimization of geometry parameters of spraying system
- determination of optimal spraying regime

Modeling results. Distributions on the axis of symmetry

Gas density, kg/m³

Gas pressure, MPa

Modeling results. Distributions on the axis of symmetry

Mach number

Density of total energy, MJ/m³

Modeling results. 2D distributions

Longitudinal velocity (u_x), m/s

Density of total energy, MJ/m^3

Modeling results

Density distribution of the particle system on the axis of symmetry
at the moment of gluing the nanocluster to the substrate. The image is rotated 90 degrees.

Conclusion

- The complex technology of supercomputer modeling the problems
  of spraying the metal nanoparticles on substrates is presented.
- A spraying model combining macroscopic, mesoscopic and
  microscopic levels is proposed. The model include:
  quasi-gasdynamics equations, convection-diffusion equations,
  Newton's equations.
- Numerical methods that combine the grid and particle methods
  have been developed.
- 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 attention!