HIERARCHICAL APPROACH TO NANODESIGN ROM THE SYSTEM THEORY VIEWPOINT

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Abstract – Hierarchy of nanosystems' simulation models are discussed from the viewpoint of the multilevel hierarchical systems' theory by S. Novikava (Aed theory).

I. INTRODUCTION

Current scientific and technological progress is usually understood in close links with the development of nanotechnology, the subject of which includes structures, processes and functions based on materials with properties defined on spatial scales 1 – 100 nm. The fundamental difficulty of nanotechnology is the fact that nanostructures are so small that it is very hard to manipulate them precisely, and simultaneously too large for direct application of precise chemical methods such as genetic engineering for their treating. Methods of simulation of them have to be both fast and precise enough for the prediction and optimization of the electronic, atomic and phase structures, functional properties and chemical behaviour of nanomaterials. Modeling of nanomaterials and nanosystems is a sophisticated task due to the fact that properties of nanomaterials are defined by interacted groups of hundreds of atoms and could hardly be computed by *ab initio* quantum mechanics (QM) methods even on supercomputers [1]. Components of nanosystems composed from such atomic groups contain millions of atoms and can be treated by molecular dynamics (MD) methods rather than QM, while the whole nanosystem can contain dozens of billions of atoms and only the finite elements' (FE) continuous approximation can be applied to it. In general system theory it is established [2] that the description of such systems have to be decomposed into interrelated description levels when at every lower level only these properties and variables of the system are calculated which are necessary for modeling it on the upper level, and, on the other hand, the upper level determines modeling tasks and constrains for calculation on the lower level. The full model represents the hierarchy of the decision making according to Mesarovich. Then the hierarchical multilevel system theory (HMST) must be used in nanosystems computing too. This approach generalizes multiscale simulation approach and corresponds to combined traditional "up-to-down" and novel "down-to-up" technologies in nanodesign.

II. S. NOVIKAVA'S AED MATHEMATICS AND NANODESIGN

Current stage of HMST is Aed theory by S.Novikava [3], which has now two main hierarchical symbolic images ${}^{\times}\alpha^{\lambda}$ and ${}^{+}\alpha^{\lambda}$ corresponding to the acts of multiplying (learning) and uniting (design) respectively. They contain the new means of control and connect the strata (directions) of A^{λ}. Aed strata are: Λ,λ–level (time), Γ,γ–statute (law, connection), P,ρ– act (process), Ω, ω – unit (state) Σ,σ – construction (contents), B, β – new time (arising level), A, α – sway (coordinator). Aed statute A^{λ} in current level λ is described by its symbol image ${}^{\times}\alpha^{\lambda}$ in following way:

$$\mathrm{A}^{\lambda} \underset{\rho}{\overset{\gamma}{\longleftrightarrow}} \left\{ \begin{matrix} \beta & & \gamma & \\ \omega & \mathrm{A} & & \lambda \\ & \rho & & \sigma \end{matrix} \right\}^{\lambda \xrightarrow[\rho]{\mathrm{A}^{\lambda}} \beta} \qquad \Lambda^{\lambda} \underset{\rho}{\overset{\gamma}{\longleftrightarrow}} \left\{ \begin{matrix} \beta & & \gamma & \\ \omega & \Lambda & & \lambda \\ & \rho & & \sigma \end{matrix} \right\}^{\lambda \xrightarrow[\rho]{\Lambda^{\lambda}} \beta} \qquad \Gamma^{\lambda} \underset{\rho}{\overset{\gamma}{\longleftrightarrow}} \left\{ \begin{matrix} \beta & & \gamma & \\ \omega & \Gamma & & \lambda \\ & \rho & & \sigma \end{matrix} \right\}^{\lambda \xrightarrow[\rho]{\Gamma^{\lambda}} \beta} \qquad \mathrm{P}^{\lambda} \underset{\rho}{\overset{\gamma}{\longleftrightarrow}} \left\{ \begin{matrix} \beta & & \gamma & \\ \omega & \mathrm{P} & & \lambda \\ & \rho & & \sigma \end{matrix} \right\}^{\lambda \xrightarrow[\rho]{\mathrm{P}^{\lambda}} \beta}$$

$$\Omega^{\lambda} \underset{\rho}{\overset{\gamma}{\longleftrightarrow}} \left\{ \begin{matrix} \beta & & \gamma & \\ \omega & \Omega & & \lambda \\ & \rho & & \sigma \end{matrix} \right\}^{\lambda \xrightarrow[\rho]{\Omega^{\lambda}} \beta} \qquad \Sigma^{\lambda} \underset{\rho}{\overset{\gamma}{\longleftrightarrow}} \left\{ \begin{matrix} \beta & & \gamma & \\ \omega & \Sigma & & \lambda \\ & \rho & & \sigma \end{matrix} \right\}^{\lambda \xrightarrow[\rho]{\Sigma^{\lambda}} \beta} \qquad \mathrm{B}^{\lambda} \underset{\rho}{\overset{\gamma}{\longleftrightarrow}} \left\{ \begin{matrix} \beta & & \gamma & \\ \omega & \mathrm{B} & & \lambda \\ & \rho & & \sigma \end{matrix} \right\}^{\lambda \xrightarrow[\rho]{\mathrm{B}^{\lambda}} \beta} \qquad \mathrm{A}^{\beta} \underset{\rho}{\overset{\gamma}{\longleftrightarrow}} \left\{ \begin{matrix} ? & & \gamma & \\ \omega & \mathrm{A} & & \beta \\ & \rho & & \sigma \end{matrix} \right\}^{\beta \xrightarrow[\rho]{\mathrm{A}^{\beta}} ?}$$

In this way all aed strata can renovate its original unit A^{λ} they have all its signs and abilities. The strata $\Lambda, \Gamma, \mathrm{B}, \mathrm{P}, \Sigma, \Omega$ are strongly connected both by their original.unit A^{λ} and by the details of their own constructions (by their new interactions). Thanks to that all aed strata may be renovated when any stratum is changed. The acts of original unit A^{λ} multiplying and their symbol images uniting lead to

the arising of the new time unit A^{β}. It contains hazy symbols in its image (they are signed by the symbol ? and they will be defined in time β).

The image ${}^{+}\alpha^{\lambda}$ (Fig.1) allows to see the acts of multiplying & uniting (learning & design), their bases, aims and connections. In Fig 1 A^{λ} - original state of aed ($A^{\lambda} \leftrightarrow \omega^{\lambda}$), A^{β} - its leading state in time λ; multiplying act ${}^{\times}\rho^{\lambda}$ of original order γ^{λ} (original statute of A^{λ}) executes learning process in the units $\omega^{\lambda\tau}$ of construction $\sigma^{\lambda\tau}$ which was created in time λ_{τ}; thanks to that the units $\omega^{\lambda\tau}$ turn into the ordinary units ω_{τ}^{λ} in the new construction σ^{λ}; uniting act ${}^{+}\rho^{\lambda}$ in σ^{λ} connects the ordinary units ω_{τ}^{λ} and creates the new sway $\omega^{\beta} \leftrightarrow A^{\beta}$; in the process ρ^{λ} the image of arising time β^{λ} has two strata - ${}^{\times}\beta^{\lambda}$ and ${}^{+}\beta^{\lambda}$ which answer to the stages of this process: ${}^{\times}\rho^{\lambda}$ and ${}^{+}\rho^{\lambda}$.

Application of HMST to nanosystems leads to hierarchical structure presented in Table 1. Every level must be split on two sublevels corresponding to classical and quantum descriptions of electromagnetic field.

TABLE 1 – Hierarchical simulation levels of nanosystems

N	Simulation level name. Basic equations	Space and time scales. Elementary unit. Number of atoms.		Values calculated at the level	Comments
6	System level. State space models $\begin{cases} \dot{\vec{x}} = \mathbf{A}\vec{x} + \mathbf{B}\vec{u} \\ \vec{y} = \mathbf{C}\vec{x} + \mathbf{D}\vec{u} \end{cases}$	100 nm - 1 m, 1 ps - 1 year. System unit, subsystem, element of system. 10^{23} atoms/mole		Transition functions, frequency responses, control algorithms, regular and stochastic regimes.	Models used in system theory and automatic control
5	Continuum level. Maxwell's and balance equations, state equations, boundary conditions	500 nm - 1 mm, 1 mcs -100 s. Continuum media element. 10^{6}- 10^{10} atoms		Electromagnetic, mechanical and thermal behavior of micro- and nanosystems' elements.	Systems of partial differential equations for averaged fields
4	Mesoscopic level. Fluctuations' dynamics on the basis of level V equations with fluctuation sources included	50 nm - 1 mcm, 50 ns -1 ms. Polycrystalline grains, granules, nanoclusters, powders. 10^{6}- 10^{10} atoms		Electromagnetic, mechanical and thermal behavior of elements, linear response theory, fluctuation-dissipation relations.	Systems of stochastic partial differential equations for fluctuated physical fields
3	Molecular dynamics level. Newton's equations	1 - 500 nm, 1ps - 50 ns	Atomic clusters, macromolecules, multiwall nanotubes. 10^{3}- 10^{8} atoms	viscosity, thermo- and electroconductivity, material constants, phase diagrams, state equations, steady state structures, phase transitions, non-equilibrium processes	Solution of Newton's equations for all atoms in thermostat
	Kinetics level. Liouville's equation	1 nm - 10 mcm, 1 ps - 10 mcs			Probability distribution densities of various order
2	Quantum statistical level. Von Neuman's equation	10 Å–100 nm, 100 fs – 10 ps Crystal unit cell, cluster in adjacent medium 10 – 1000 atoms		Inter-cluster interaction, cluster surfaces, stochastic energy spectrum	Statistic operator or density matrix
1	**Quantum mechanical level**. Schrödinger's equation	0.1-20 Å, 1-1000 fs. Molecule, isolated cluster. 10 – 100 atoms		Interatomic interaction potentials, electronic subsystem distribution density	*ab initio* models, molecular orbitals' theory, DFT

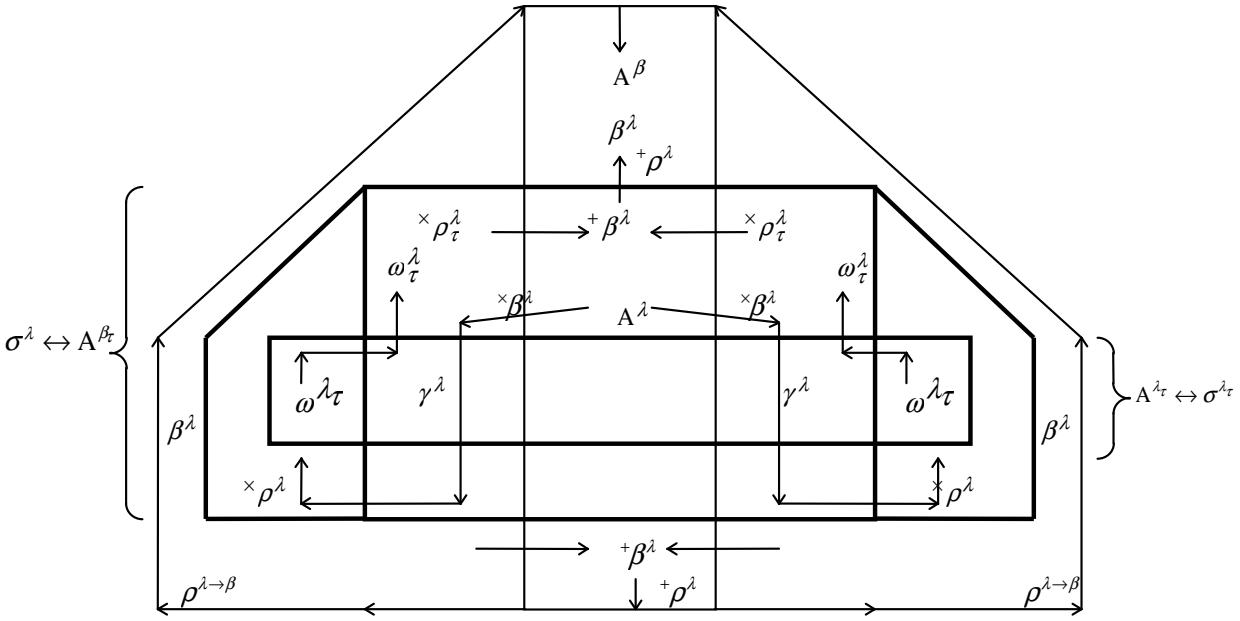

Figure 1 – Symbolic image of aed

III. Conclusion

In this paper the we discuss the hierarchical approach to nanodesign and present its formal realization on the basis of the aed theory. Description of nanosystems have to be decomposed into interrelated levels when at every lower level only these properties and variables of the system are calculated which are necessary for modeling it on the upper level, and, on the other hand, the upper level determines modeling tasks and constrains for calculation on the lower level.

References

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