MULTI-SCALE PRODUCT DESIGN AND LIFECYCLE SIMULATION SYSTEM FOR NANO PRODUCT DEVELOPMENT

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It is important for product designer to get overview and forecast of the property and the influence of designing product by computer simulations. In order to support product designer and material designer, multi-scale product design and lifecycle simulation system is proposed. Multi-scale product design and lifecycle simulation system consists of multi-scale product design and simulation (MPDS) sub-system and product lifecycle simulation (PLS) sub-system. Multi-scale product design and lifecycle simulation system carries out continuous multi-scale CAD/CAE from micro/nano scale level to human scale level, and carries out product lifecycle simulation of designing product or material. Multi-scale spatial model of MPDS sub-system is a computational model of physical space, an interface and a bridge between multi-scale CAE simulations. PLS sub-system is designed from the point of view of the interactions of subjects and growth and decline of subject caused by designing product or material in the flow of physical, social, and economic entities. A subject of PLS sub-system represents factory, company, shop, organization, group of people, or individual. MPDS sub-system and PLS sub-system are implemented with message passing interface (MPI).

1. Introduction

Product designers are demanded to harmonize technical, economic, social, and environmental aspects of designing product. It is important for product designer to get the overview and the forecast of the property and the influence of the designing product by computer simulations. In order to support future product designer and material designer, a framework of multi-scale product design and lifecycle simulation system is proposed. Figure 1 shows the framework of multi-scale product design and lifecycle simulation system. Multi-scale product design and lifecycle simulation system consists of multi-scale product design and simulation (MPDS) sub-system and product lifecycle simulation (PLS) sub-system. Concept of MPDS sub-system is an expansion of concept of current CAD/CAE system. Multi-scale products from micro/nano scale level to human scale level are designed continuously in the MPDS sub-system. Multi-scale spatial model of MPDS sub-system is a computational model of physical space and a bridge between multi-scale simulation modules. Concept of PLS sub-system is an expansion of concept of current LCA system. PLS sub-system carries out product lifecycle simulation and evaluation of designing product.

PLS sub-system is designed from the point of view of the interactions of subjects and growth and decline of subject caused by designing product or material in the flow of physical, social, and economic entities.

A subject of PLS sub-system represents factory, company, shop, organization, group of people, or individual. The information of designing product is projected into PLS sub-system as a structured token made by MPDS sub-system.

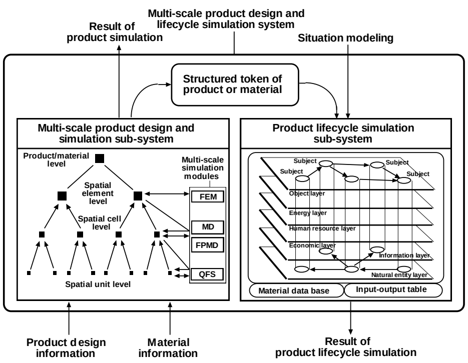

Fig. 1 Concept of multi-scale product design and lifecycle simulation system

2. Framework of MPDS Sub-system

2.1 Model of Physical Space

Figure 2 shows the framework of MPDS sub-system. Multi-scale spatial model is a model of physical space. Multi-scale spatial model consists of attribute distribution space, thermodynamics quantities distribution space, energy distribution space, particle space, atomic nucleus space, electron distribution space, potential distribution space, lattice space, multi-scale spatial tree, and spatial samples. The attribute distribution space is a macro-scale level space. The thermodynamic quantities distribution space is a meso-scale level space. The energy distribution space is a meso-scale level space. The particle space, the atomic nucleus space, the electron distribution space and the lattice space are micro/nano-scale level spaces. The particle space consists of the kind, the coordinates and the momenta of molecules. The atomic nucleus space and the electron distribution space are derived from the particle space. The lattice space is a model of quantum field.

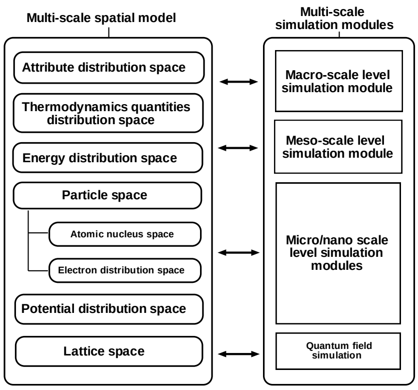

Fig. 2 Framework of MPDS sub-system

2.2 Multi-scale Spatial Tree

Figure 3 shows the concept of multi-scale spatial tree of MPDS sub-system. Product and material of MPDS sub-system consist of spatial elements represented by rectangular solid. Spatial element, spatial cell, and spatial unit are represented by rectangular solid. Spatial unit consists of a set of spatial nodes.

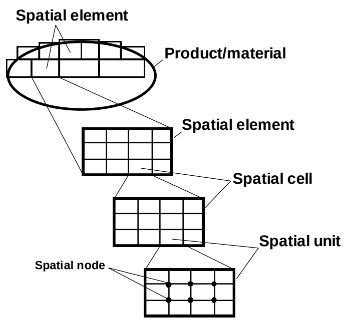

Fig. 3 Concept of multi-scale spatial tree

Figure 4 shows the detail of multi-scale spatial tree. Product and material of MPDS sub-system include numbers of spatial element. Spatial element includes attribute distribution space, thermodynamics quantities distribution space, energy distribution space, and reference numbers of spatial cell. Spatial cell includes particle space, atomic nucleus space, electron distribution space, potential distribution space, and reference numbers of spatial unit. Spatial unit includes the information of lattice space. Product or material of MPDS sub-system consists of origin and direction angles of rectangle solid of product or material, the number of spatial elements of product or material, and the reference number of spatial samples for spatial elements. Spatial element consists of origin, direction angles, and size of rectangular solid of spatial element, the number of spatial sample for attribute distribution space, the number of spatial sample for thermodynamics quantities distribution space, the number of spatial sample for energy distribution space, and the reference numbers of spatial cells. Spatial cell consists of origin, direction angles, and size of rectangular solid of spatial cell, the reference number of spatial sample for particle space, the reference number of spatial sample for atomic nucleus space, the reference number of spatial sample for electron distribution space, and the reference numbers of spatial units. Spatial unit consists of origin, direction angles, and size of rectangle solid for spatial unit, and the reference numbers of spatial samples for lattice space. Atomic nucleus space and electron distribution space are derived from the information of particle space. Atomic nucleus space and electron distribution space include the information for first principle molecular dynamics (FPMD) of multi-scale simulation modules.

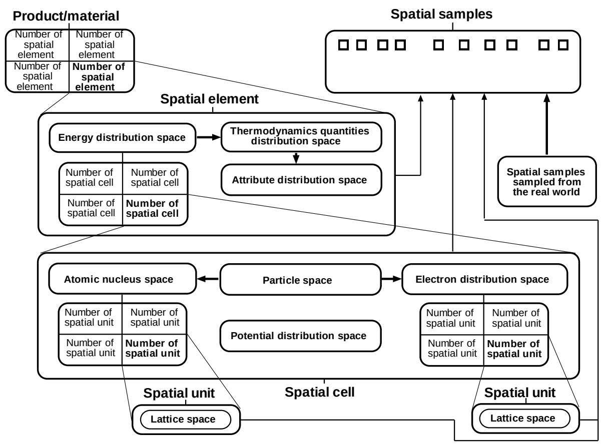

Fig. 4 Detail of multi-scale spatial tree

2.3 Distribution Spaces

Attribute distribution space, thermodynamics distribution space, energy distribution space, and potential distribution space are distribution spaces. The distribution space is represented by distribution surfaces. The distribution surface of distribution space is generated by spatial interpolation.

2.4 Particle Space

The particle space includes the information of molecules for molecular dynamics (MD) simulation of multi-scale simulation modules. Particle space consists of size of rectangular solid of particle space and the information of molecules.

2.5 Lattice Space

The lattice space of MPDS sub-system is a model of quantum field for quantum field simulation. A particle of the lattice space is represented by a spatial token. Figure 5 shows a node of lattice space. A spatial token is received and stored in a spatial node of the lattice space. Then, the spatial token is sent to the neighboring spatial node. A spatial token propagates in the lattice space. The lattice space is a modified cellular automata with depth (Figure 6). The node of the modified cellular automata with depth has communication network layers.

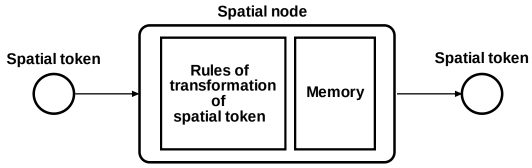

Fig. 5 Spatial node of lattice space

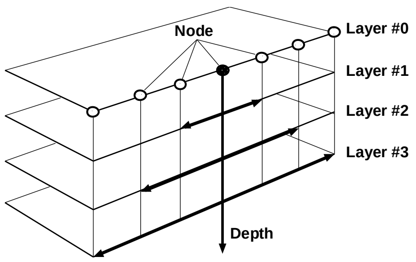

Fig. 6 Modified cellular automata with depth

2.6 Multi-scale Simulation Modules

The candidate of the macro-scale simulation module is FEM (Finite Element Method). The candidates of the meso-scale and micro-scale level simulation modules are MD (Molecular Dynamics) simulation and FPMD (First Principle Molecular Dynamics) simulation. The lattice space of MPDS system is a platform of quantum field simulation.

2.7 Spatial Sample

Spatial sample is a master and a candidate of space referencing by the spaces of multi-scale spatial model. A spatial sample is assigned repeatedly. A spatial sample is made with character string expressing the information of the space. A spatial sample is made from the result of simulation or the sampled data from the real world.

3. Implementation of MPDS Sub-system

Figure 7 shows the implementation method of MPDS sub-system in multi-scale process environment. The nodes of the lattice of spatial element handle multi-scale spatial tree. The nodes of the lattice of spatial element are implemented with processes. The multi-scale spatial tree is stored in a common file. Each node of the lattice of spatial cell includes MD and FPMD simulation modules. Spatial unit is a lattice space. FEM, lattice of spatial cell, and spatial unit are multi-scale simulation modules.

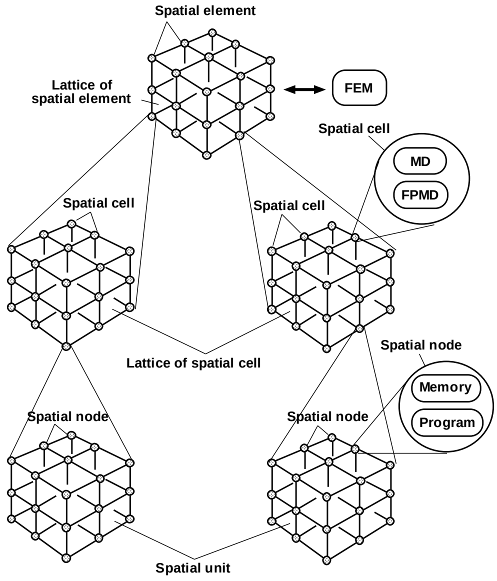

Fig. 7 Implementation method of MPDS subsystem in multi-process environment

4. Framework of PLS Sub-system

4.1 Subject and Environment

The product life cycle simulation (PLS) sub-system is designed from the point of view of the interactions of subjects and growth and decline of subject caused by designing product or material in the flow of physical, social, and economic entities.

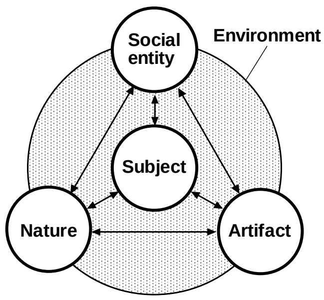

Fig. 8 Subject and environment

4.2 Concept of PLS Sub-system

A subject of PLS sub-system represents factory, company, shop, organization, group of people, or individual in the environment. Figure 9 shows the concept of PLS sub-system. PLS sub-system consists of 6 layers of sub-systems, (1) object sub-system represents products, parts, assemblies, materials, and physical entities, (2) energy sub-system represents energy supply, (3) human resource sub-system represents managers, designers, engineers, workers, clerks, and users, (4) economic sub-system represents capital and money flow, (5) information sub-system represents technical information, merchandise information, and market information, and (6) natural entity sub-system represents inartificial objects in nature.

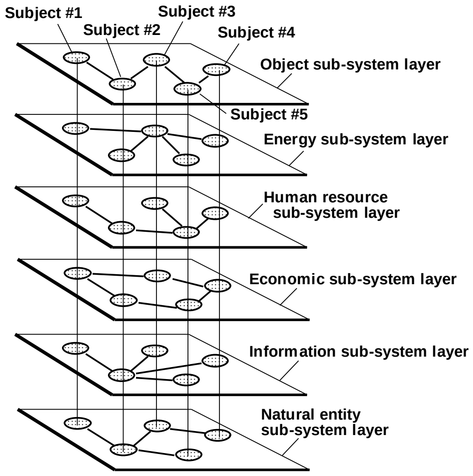

Fig. 9 Layer structure of PLS sub-system

A subject changed by the flow of physical, social, and economic entities on the layers makes new subject connecting on each sub-system layer. Physical, social, and economic entities are represented by structured tokens. The phenomena of meeting and parting of physical and social entities are represented by structured tokens. Design information consists of the structure and the processing methods of product or material. Design information is represented by structured token. A structured token occurs malfunction and recovery of a subject. The mechanism of malfunction and recovery of subject simulates the hazard against subject caused by physical, social, and economic entities. The estimation of environmental impact of designing product or material is carried out based on the gathered calculated inventory data of all subjects. The estimation of designing product or material is measured by growth and decline of subject.

4.3 Physical, Social, and Economic Entities

Figure 10 shows the meeting and parting phenomena of physical, social, and economic entities represented by the structured token.

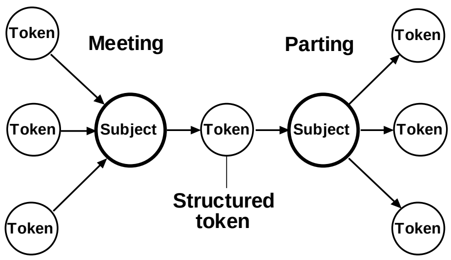

Fig. 10 Representation of behavior of entities by tokens

5. Implementation of PLS Sub-system

5.1 Representation of Subject

Figure 11 shows the representation of subject and the flow in subject. A subject consists of matrices and storage of structured tokens. A subject receives the structured tokens from the layers of sub-systems. The structured tokens transformed by the subject are sent to another subject. Selection of acceptable structured token is made with the entity selection matrix. The range checking of structured token is made with the entity range check matrix. The accepted structured token is converted to event. The event generates the related events and the destination subjects with the event network matrix. The quantity of entity related to the event is calculated with quantity calculation matrix.

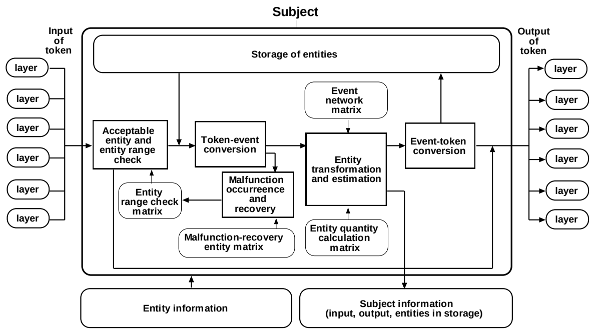

Fig. 11 Representation of Subject

5.2 Components of Structured Token

Physical, social, and economic entities are represented by structured tokens. Figure 12 shows the components of structured token with entity structure information. The entity structure information is variable length. The detail of entity including attributes, processing methods, and structure is described in the entity structure information.

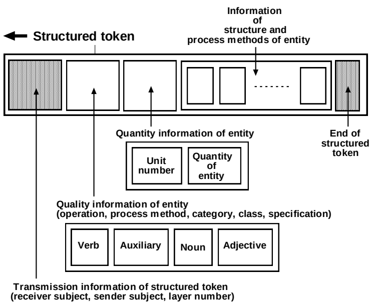

Fig. 12 Components of structured token

When the structured token occurring malfunction of subject is found in a subject, the entity selection matrix and the entity range check matrix of the subject are modified by the information of the structured token. Then, the input of the subject is changed. On the contrary, when the structured token recovering from the malfunction of subject is found in a subject, the entity selection matrix and the entity range check matrix of the subject are modified by the information of the structured token. Then, the input of the subject is recovered. The mechanism of malfunction and recovery of subject represents the hazard against subject caused by entity.

6. Conclusions

Necessity of multi-scale product design and lifecycle simulation system for product designer and material designer is indicated.

The framework and the implementation methods of multi-scale product design and lifecycle simulation system are proposed.

Nano product and chemicals have not only high performance but also potential hazard to human and environment. Multi-scale product design and lifecycle simulation system aims to find out and prevent the potential hazard to human and environment of designing product.

REFERENCES

1. Sakita, K., "Multi-scale Product Design and Lifecycle Simulation System for Environmentally Conscious Product Design", Proceedings of TMCE2010, Vol. 2, Ancona, Italy, 1211-1221, 2010.
2. Raabe, D., "Computational Material Science", Wiley-VCH Ve rlag GmbH Weinheim, Germany, 1998.
3. Okazaki, S., "Fundamental of Computer Simulation", Kagaku-dojin Company Ltd. Kyoto, Japan, 2003.
4. Tukada, M., Yamauchi, J., Kamimura, H., Kashiwagi, H., Mor okuma, K., "Material Design and Simulation", Saiensu-sha Pu blishing Company, Tokyo, Japan, 1993.
5. Ueda, A., "Molecular Simulation from Classical to Quantum Method", Shokabo Book Company, Tokyo, Japan, 2005.
6. Mori, H., Kuramoto, Y., "Dissipative Structure and Chaos", Iwanami Book Company, Tokyo, Japan, 2006.
7. Kuramoto, Y., "Bridge between Micro Scale and Macro Scale", Iwanami Book Company, Tokyo, Japan, 2002.
8. Jammer, M., "Concepts of Space", Harvard University Press, U. S. A., 1969.
9. Prigogine, I., Kondepudi, D., "Thermodynamics", Editions Odi le Jacob Paris, France, 1999.
10. Sunada, T., "Statistical Mechanics and Thermodynamics from Point of View of Mathematics", Iwanami Book Company, Tok yo, Japan, 2004.
11. Kubo, R., "Statistical Mechanics", Kyoritsu Publishing Compa ny Ltd. Tokyo, Japan, 2006.
12. Greiner, W., "Quantum Mechanics – An Introduction", Spring er-Verlag Berlin HeidelBerg, Germany, 1989.
13. Sakurai, K., "Light and Quanta", Tokyo-kyogakusha Company Ltd., Tokyo, Japan, 1998.
14. Aihara, H., "Physics of Elementary Particles", University of T okyo Press, Tokyo, Japan, 2006.
15. Ninomiya, M., "Lattice Space-time and Gravity", in "Physics a nd Mathematics of Field Theory", Saiensu-sha Publishing Com pany, Tokyo, Japan, 1991.
16. Adachi, Y., "Introduction to Entropy Assessment", Ohmsha Publishing Company, 1998.
17. Adachi, Y., Matsuno, Y., Daigo, I., Takiguchi, H., "Environmental System Engineering", University of Tokyo Press, 2004.
18. Murata, T., "Analysis and Application of Petri Net", Kindai-kagaku-sha Company Ltd., 1992.
19. Watanabe, K., "Foundation of Parallel Processing", Corona Pu blishing Company, Tokyo, Japan, 1991.
20. Gropp, W., Lusk, E., Thakur, R., "Using MPI-2: Advanced Features of the Message-Passing Interface", MIT Press, U. S. A., 1999.
21. Yokoyama, H., "Nano Materials Science", Ohmsha Company Ltd., Tokyo, Japan, 2004.