Simulation and Visualization in Cognitive Nanoinformatics

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Abstract—Features of Cognitive Informatics for nanoscale science and engineering are discussed. An approach using the fundamental principle of quantum mechanics and the principle of quantization of information is proposed. We illustrate our approach for distributed MEMS case study.

Keywords—Nanoinformatics, cognitive science, ontology, simulation, visualization, MEMS.

I. INTRODUCTION

Nanoinformatics is an application of e-Science to nanoscale science and engineering [1]. Nanoinformatics includes the following activities: data collection, management, storage, modeling, simulation, and results analysis. All mentioned above activities serve to extract useful information relevant to nanoscale science and engineering for the further scientific research.

In despite of recent outstanding results in nanoscale science and engineering an impossibility to observe nanoobjects by human eyes results in cognitive problems in nanoscale research activities.

In [2] two approaches to cognitive environment for nanoinformatics have been discussed. The first approach is based on mind map visualization techniques. A mind map is a reflection of the thinking about a topic [3]. The map has radial structures with the central image. Mind maps are effective technique to help a human mind to keep ideas generated during some discussion, e.g. during brain storming. Another approach is based on concept maps. Concept maps visualization techniques are based on concepts and links between them [4]. Concept maps represent a systematic view and can have several conceptual centers. Mind maps and concept maps are applied in different areas including higher education, business, government etc.

In the paper we discuss our experience in the application of these cognitive techniques in Nanoscale science and engineering. In our discussion, we use notations of Cognitive Informatics [5] that are based on matter, energy, and information.

We also discuss features of computer simulation in nanoscale science and engineering and its role in Cognitive Nanoinformatics tools.

The rest of the paper is structured as follows. Section 2 is about Mind Maps and Concept Maps visualization techniques and the corresponding mapping software. We discuss features of computer simulation in nanoscale science and engineering and techniques that are used to visualize simulation results in Section 3. Section 4 reviews related works in the field of Cognitive Informatics. Section 5 presents our preliminary results in Cognitive Nanoinformatics. Finally, conclusions are derived in Section 6.

II. MAPS VISUALIZATION TECHNIQUES

A. *Mind and Concept Maps Visualization Techniques*

Mind maps have been proposed by T. Buzan in the 1970s [3]. His research was based on the pioneering split-brain research by R. Sperry et al. The main outstanding outcome of their research was that a human brain works better with key words and direct associations. Left and right brain hemispheres support different functions. Logical functions are supported by the left hemisphere, while creativity is supported by the right hemisphere. Therefore, special techniques to exploit both hemispheres are required.

T. Buzan formulated the following rules of mind maps drawing. First of all, the main definition (one or two words) has to be selected. The main definition is placed in the center as the central image. Then the major associated words are selected. They radiate from the center node. Hierarchical structure is strongly advised. More important associated words are placed with branches to the center. The lower level of hierarchy has branches to higher level of hierarchy. Visual images and figures are strongly recommended to be used in mind maps visualization technique.

Mind maps are used to relate objectives, capture ideas and information. This radiant, non-linear structure is a natural function of the human mind. The mind maps visualization techniques use the whole brain resources and support multidimensional thinking. In addition, personal learning, memory and creativity are expected to be enhanced.

Concepts maps were proposed by J. Novak in the 1970s [4]. These techniques are based on the assimilation theory of D.

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Hint: Try MindMeister for iPhone, iPad or Android. View

Fig. 1 An example of a mind map drawn in Mind Meister

Ausubel. The maps use concepts and relations between the concepts. In comparison to mind maps, the concept maps represent a systematic view of a research object and use a free structure with many clusters and their associated words. It should be noted that concepts maps potentially contain more information in comparison to mind maps and can be used for ontology building. Hierarchical structure of concept maps is strongly recommended. No more than 25 concepts in one layer is used for simplicity and better knowledge transfer.

Mathematically, both mind maps and concept maps represent a graph with additional information on vertexes and edges. Therefore, the graph theory can be applied to analyze features of these specific graphs (number of vertexes, edges, the chromatic number of a graph etc.).

Mind and concept maps visualization techniques are effective in many areas. In this paper, our focus is on application of the mind maps and concept maps visualization techniques in Nanoinformatics. Their applications add cognitive elements to Nanoinformatics. Information systems that are based on mind and concept maps obey the laws of Cognitive Informatics that have been established in [5].

B. Mapping Software

Mind maps and concept maps can be created manually and through the use of software. Currently commercial and free mapping software with the capability to create digital versions of maps is available. Some popular mapping tools are discussed below.

MindMeister [6] is a leading online mind mapping software. Free basic restricted version is available after registration. It runs on Microsoft Windows, Linux, and Mac operating systems. MindMeister has many export and import capabilities. Collaboration in real-time with team members is supported. Fig. 1 demonstrates an example of a mind map drawn in Mind Meister.

Compendium [7] is a free tool that uses the mapping of ideas. The tool supports not only a creation of mind and concept maps, but argument and dialogue maps. It is written in Java and runs on Microsoft Windows, Linux and Mac operating systems. It widely used in Open University (UK) in research work and course development.

The IHMC Cmap Tools [8] is a free concept mapping software written in Java. It is the most popular free concept mapping software. It runs on Microsoft Windows, Linux and Mac operating systems. Its interface can be easily used for several applications including Web applications. An example of a concept map drawn in the IHMC Cmap Tools is shown in Fig. 2.

III. SIMULATION AND VISUALIZATION IN NANOSCALE SCIENCE AND ENGINEERING

Nanoinformatics is a new research area that uses knowledge in different disciplines: mathematics, informatics, physics, chemistry etc. It is remarkable that manufacturing of nanoobjects is very expensive. Therefore, simulation plays a crucial role during design process [9].

A. Simulation

In nanoscale science and engineering models of all levels are used including [10]:

- continuum approximation (classic models);
- semi-classic models;
- *ab initio* quantum mechanical models.

Therefore, many tools are used for nanosystems simulation.

Classical models include finite difference methods, finite elements methods and boundary elements methods [11]. The finite difference methods are numerical methods that are not computational expensive in comparison to other two methods. However, their accuracy is lower in a comparison with more computational expensive finite elements methods and boundary elements methods. The boundary elements methods are more efficient in a comparison with the finite difference methods and finite elements methods. However, their applications require huge computation efforts. This deficiency hinders their applications in engineering practice.

The finite elements methods are a compromise between

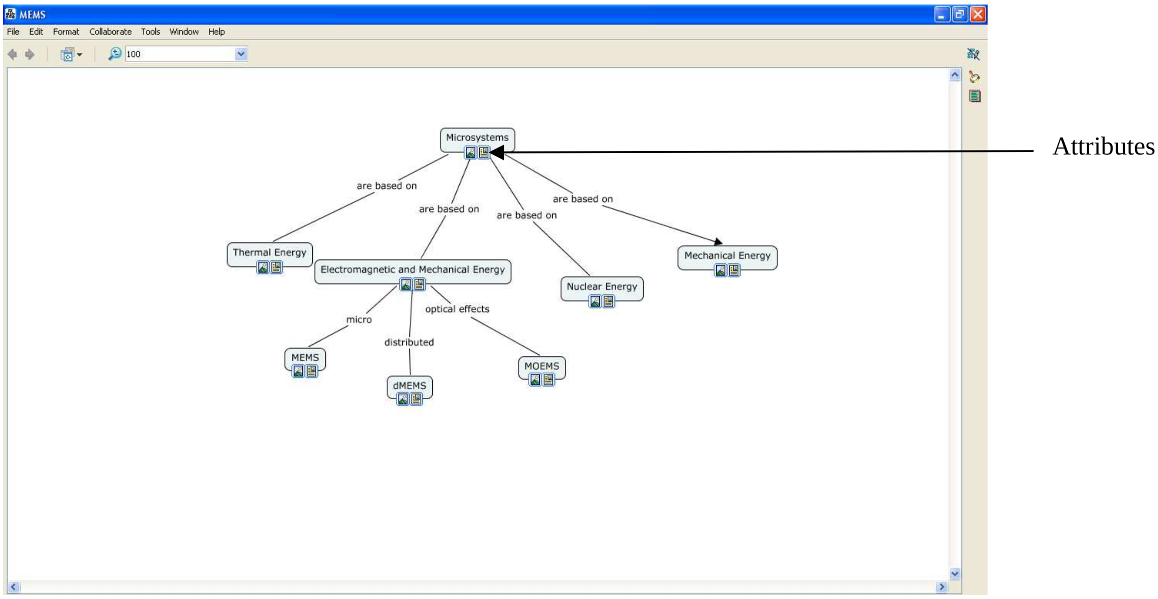


Fig. 2 An example of a concept map drawn in IHMC Cmap Tools

accuracy and computational efforts. They are widely used in many commercial tools, e.g. ANSYS, to simulate different physical effects. The ANSYS Multiphysics [12] is used for simulation in different areas, including automotive, space industry etc. The tool can be used for simulation of nanosystems as well [11]. It supports two main methods for multi-physics simulation: the sequential method and direct method. Both methods represent the finite elements methods. The sequential method is used in weak coupling cases while the direct method is used in highly nonlinear cases.

The first principle approach is based on the basic equations governing matter and energy. It can applied to any physical systems. These methods are correct and predictive. However, it is really impossible to receive inputs that are required for these methods, e.g. Gibbs energies, for real-world cases. Moreover, the computation cost is high.

Monte Carlo simulations represent an effective method that is based on simplified or semi-classical models [10]. It is more flexible in comparison with the first principle methods. However, its accuracy is lower. The computation cost is a compromise in comparison with the first principle approach and continuum approximation methods.

Simulation for real-world problems often requires multi-scale models. In this case one part of the system is simulated using the first-level principles and the rest is described in approximate ways, using semi-classical models and/or classical models. However, links between different levels are unclear for any materials and further research activities are required for novel multi-scale methods.

B. Visualization

Research in nanotechnology hinders by tiny sizes of nanosystems. Visualization is a crucial component in effective design of nanosystems because virtual images of nanosystems can be created in virtual reality. These images can be drawn through commercial tools or simulation results can be collected and then visualized.

Mostly nanoscale simulations generate scalar data, vector data or a combination of the two. As a result a visualization tool has to support these data formats.

Microsoft Visio [13] is one of visualization market leader and can be used to draw 3D models of nanosystems, technological operations etc. It runs on Microsoft Windows operating system only. Specific templates for the both mentioned above mapping visualization techniques and nanosystems simulations are not provided.

The postprocessors in ANSYS Multiphysics [12] were designed to display simulation results. Contour displays, vectors displays, and graph displays are used to review simulation results. It should be noted that the tool supports visualization of simulation results for continuum models only. In the general case it is impossible to apply the tool for nanosystems simulation and design.

The Visualization Toolkit (VTK) [14] is a free visualization library written in C++. It can be used for several applications including nanoscale science and engineering visualization tasks. VTK supports different visualization methods including scalar and vector methods.

The NanoVis [15] library has been designed to handle a visualization of nanoscale simulations including a visualization of scalar and vector data. The library is an open source code and requires NVIDIA graphics acceleration.

IV. RELATED WORKS

A lot of information available for a researcher in nanoscale science and engineering requires novel approaches to manage this information space. New information management tools and devices introduced to market and an engineer has to use these new tools in order to be competitive.

In [5] the theoretical foundations of cognitive informatics have been discussed. It was shown [5] that matter (*M*) and energy (*E*) are used to model the physical world (PW) while information(*I*) is used to model the abstract world (AW). It should be noted that the natural world is a dual world. One aspect is the physical world while the other is the abstract world. The natural world model is given as follows [5]:

$$NW = PW \; // \; AW = F(I, M, E), \tag{1}$$

where // denotes a parallel relation between two worlds: physical and abstract worlds;

F is a function that determines the natural world and relations between information, matter, and energy (*I-M-E* model).

Parallel relations between the physical world and the abstract world play a crucial role in a human mind. Information serves as a bridge in the connecting the physical and abstract worlds.

In [5] the principle of transformability between *I-M-E* states was described by the following generic functions:

$$I = f_1(M), \tag{2}$$
$$M = f_2(I), \tag{3}$$
$$I = f_3(E), \tag{4}$$
$$E = f_4(I), \tag{5}$$
$$E = f_5(M), \tag{6}$$
$$M = f_6(E). \tag{7}$$

A. Einstein found the relations between matter and energy (functions f_5 and f_6) in the form

$$E = Mc^2, \tag{8}$$

where *c* is the speed of the light

$$c = 3 \times 10^8 \, m / c.$$

It seems to be that the relations between *M-E-I* and possible solutions for functions f_1 - f_4 are one of the fundamental problems in Cognitive Informatics.

The systematic approach to computer aided design simulation has been considered in [16]. It was shown that a creativity of a designer is enhanced by means of virtual images exploitation. A role of visual thinking in the abstract world has been emphasized in [16] as well.

Mapping techniques have attracted attention of many researchers in information management. In [17] several applications of Compendium [7], a free mapping tool, have been discussed. It was shown benefits of the open education resources sharing through maps. Two case studies include two courses of the Open University (UK), namely the Exploring Psychology's Context and History Unit by the Faculty of Social Sciences and the Project Management Unit by the Open University Business School. However, information management skills for Engineering and Nanoinformatics applications are not discussed in details.

In [18] applications of mind maps to production engineering and management education have been discussed. Mind map visualization techniques have been used in course "Introduction to Electricity and Electronics" as well [19]. In the case study [19] mind maps have been created both manually and through Mindjet software. It was shown [19] that students results have been improved slightly. However, it is more important that long-term knowledge has been enhanced. However, some electrical engineering students indicate that these techniques were not effective for them. In [20] assessment procedures based on concept maps have been outlined. It was proposed to give the highest scores to the maps with a large number of concepts, links and an extensive hierarchy. The proposed methodology has been tested for instruction in Electronics.

In [21] a role of knowledge management and knowledge representation has been discussed. It was shown that different types of knowledge require different type of representations. Links with three other research fields: logic, ontology, and computation have been considered in details. The following classification of map items has been proposed. The crossroads have been defined as items connecting different fields. The roads connect items belonging to one research area, e.g. chemistry. The leaves are items including some associations, usually individual images.

The promising area in Nanoscale Engineering has been outlined in [22]. They are biotechnology (biomedical wires, biosensors etc.), energy (solar cells, supercapacitors etc.), medicine (personal care, minimally invasive surgery etc.) and etc. It was shown that these multi-field applications require multi-filed approaches to simulation of nanosystems.

In [23] fundamental issues in Nanoinformatics have been formulated. It was shown that ontology level is the most effective for knowledge representation in Nanoinformatics.

The ontology represents knowledge by means of a set of concepts and relations between them. Mathematically, ontology is given as follows:

$$O =< A, B, C >, \tag{9}$$

where *A* is the set including all concepts in the ontology;

B is the set including all relations between all concepts in the ontology;

C is the set representing all axioms for the sets A and B.

A role of cognitive visual environments in Nanoinformatics has been discussed in [23] as well. It was shown that the multi-filed nature of research in nanoscale science and engineering requires cognitive approaches to knowledge management.

V. dMEMS CASE STUDY

A. General Remarks

Mapping visualization techniques are based on recent results in brain research. Creativity is enhanced with the maps visualization techniques. Team communication is more effective with visualization tools including mind maps and concept maps visualization techniques as well.

In general, both mind maps and concept maps visualization techniques can be used in cognitive information systems. However, concept maps visualization techniques storage data and can be used to create ontology. We will discuss concept maps applications in Nanoinformatics below.

It is remarkable that in the general case concepts in (9) belong to the abstract world and the physical world. Therefore, the corresponding set *B* represents relations between *I-M-E* and transformations between *I-M-E* states.

This knowledge representation model transforms equations (2)-(7) to a graph model. We propose that for nanoscale science and engineering equations (2)-(7) are given as follows

$$\begin{aligned} I &= \psi(M, E), \\ E &= f_5(M), \\ M &= f_6(E), \end{aligned} \qquad (10)$$

where ψ is a generic function, depending from the functions (2) - (7).

Equations (10) have to be used in Cognitive Nanoinformatics when simulations using *ab initio* and semi-classical models are performed. In some particular cases equations (2)-(7) can be used for simulations using continuum models. However, we propose to use equations (10) in Cognitive Nanoinformatics because of reasons of generality.

Equations (10) are correct according to the foundation principle of quantum mechanics and the principle of quantization of information [24]. In [24] it was formulated that an elementary system carries 1 bit of information. Therefore, (10) allows us to avoid multi-valued functions.

Concepts in ontology (9) contain different attributes (Fig. 2) such as tables, images, simulation results, etc. These attributes can be used in visual analytics, e.g. to observe trends in design space, as well. Usually a designer uses simulation results one time for design purposes. Then these simulation results are destroyed. This engineering practice is valid for simple design cycles. However, for nanoscale science and engineering novel approaches that are based on e-Science are required. We propose to collect data as attributes of the corresponding concepts.

We illustrate our approach for distributed MEMS case study below.

B. Simulation and Visualization: dMEMS case study

Distributed MEMS (dMEMS) are the key enablers of the Internet of Things. They are simulated using models of two levels.

The behavioral level dMEMS models are simple but less accurate. In the general case ordinary differential equations are used for this level.

The multi-field dMEMS models are more accurate but more computationally expensive. Partial and ordinary differential equations are used for this modeling level.

We propose to save the behavioral and the multi-field dMEMS models and simulation results as attributes of the corresponding concepts for our case study.

In our case study we have chosen the following attributes:

- VHDL-AMS models of our dMEMS;
- 3D models in IGES format;
- information about a finite element that has been chosen for meshing (visual images, a name according to the ANSYS elements library, number of nodes, freedom degrees, etc.);
- ANSYS binary data base including 3D model, material properties, and a finite element model;
- simulation results (tables, visual images);
- trends in variables;
- additional information about the dMEMS.

It should be noted that the availability of 3D model in IGES format allows a designer to use this model in different CAD tools.

It is remarkable that one attribute, namely the ANSYS database contains an information about the abstract world (3D model, a model for simulation) and an information about the physical world (matter properties, including Young module, temperature coefficients etc.) according to (10).

Our system was implemented in IHMC Cmap Tools. Figs. 3, 4 illustrate our distributed MEMS (dMEMS) case study. We simulate our dMEMS using modal analysis options of ANSYS [12]. We have chosen silicon as material for our dMEMS. A 3D model of our dMEMS is shown in Fig. 3, a. Another attribute (Fig. 3, b) represents a visual image of the finite element that has been chosen for finite elements analysis. The next attribute (Fig. 4, a) represents finite element model for our case study. The last attribute (Fig. 4, b) visualizes trends in eigen frequencies variations because of technological uncertainties (Δ=± 2 μm).

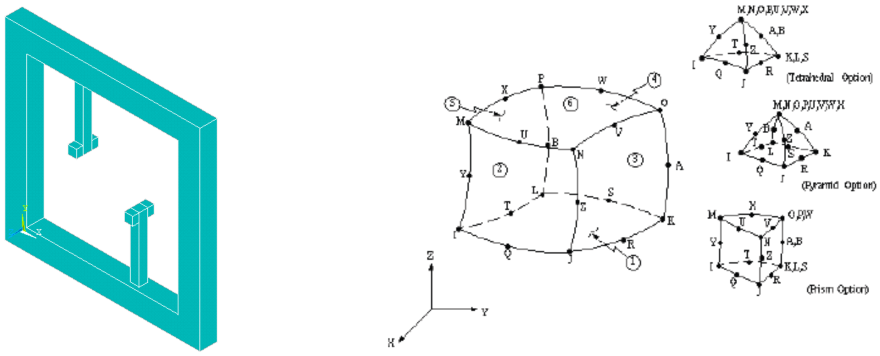
The data mentioned above can be used for design goals (e.g., trends, Fig. 4, b) and for other simulation runs (e.g., 3D model (Fig. 3, a) and finite elements model (Fig. 4, a)).

It should be noted that out approach can be applied for nanoelectromechanical systems (NEMS) as well without loss of generality.

VI. CONCLUSION

The paper has presented features of Cognitive Informatics for nanoscale science and engineering.

Two visualization techniques that are based on recent results in brain research have been discussed. Mind maps can be used to enhance engineering outcomes by means of own mind images generated during a discussion, while concept maps can



(a) (b)

Fig. 3 An example of attributes for our dMEMS case study (a) 3D model of the dMEMS, (b) a visual image of the finite element and its options

be used for text mining and enhancing metacognition. It is remarkable that mind maps and concept maps add cognitive elements to scientific process. Their application in Nanoinformatics software tools enhance creativity and team efficiency.

A short review of mapping software was given. Free, commercial and online software can be used in Nanoscale science and engineering. It seems to be that the most effective in the context of a globalization is online software because it provides a collaborative cognitive environment.

In the paper, we have discussed some issues concerning a role of simulation and visualization in Nanoinformatics. The distinguish feature of nanoscale science and engineering is the use of models of all levels from *ab initio* models to continuum models. It results in multi-scale modeling in the general case. Visualization is an important component in Nanoinformatics systems as well. The general purposes and special nanoscale science and engineering tools and libraries have been discussed.

The theoretical foundations of Cognitive Informatics have been outlined and adapted for nanoscale science and engineering. It was shown that in Cognitive Nanoinformatics more general models have to be used because of the basic principles of quantum mechanics. The information content of the elementary system is limited to 1 bit of information. In order to avoid multi-valued functions in (2)-(7) problems model (10) has been proposed.

Our approach has been illustrated for distributed MEMS case study. It was shown that the corresponding concepts contain information about energy and matter simultaneously. It seems to be impossible to divide matter from energy in the general case in order to derive functions (2)-(7).

It should be noted that our knowledge base is discrete because technologically all possible sizes of dMEMS are fixed and dictated by a chosen technological process and equipment. This discrete character of design space for our dMEMS case study simplifies significantly optimization process.

The principle of quantization of information [24] allows us to find a solution of the problems that have formulated in [25]. In the general case the classical computers are unable to simulate a quantum system [25]. However, an elementary system carries 1 bit information similar to the simplest cell of a classic computers. Therefore, transformability between information-matter-energy in (10) is possible for one-bit level.

Finally, in order to simplify links between concepts in an ontology more complex knowledge representation models can be used, e.g. information granules, genotype-phenotype knowledge representation [26].

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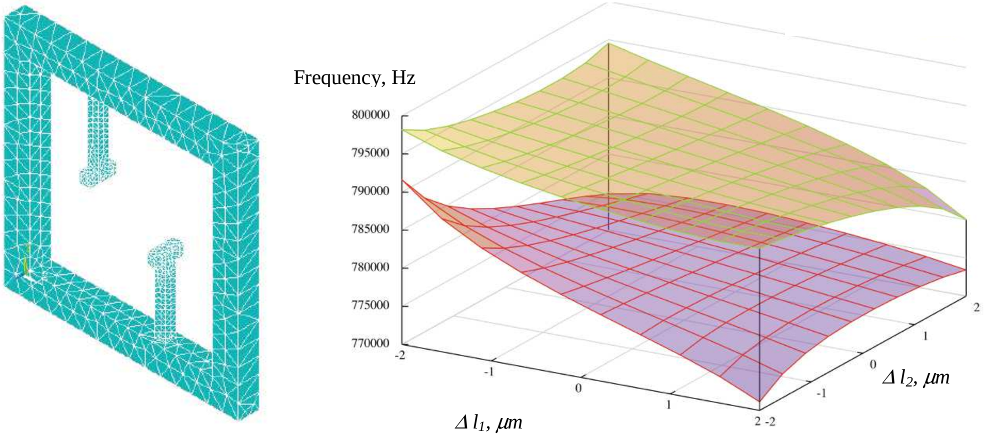

(a) (b)

Fig. 4 An example of attributes for our dMEMS case study (a) Finite element model of the dMEMS (b) Trends in eigen frequencies variations

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