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Virtual Modeling Laboratories for Knowledge Integration and Creation

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ABSTRACT

This paper deals with one of the key issues of modeling work: how model-based complex problem solving can efficiently exploit huge amounts of knowledge available on a countless number of interconnected computers. Solving complex problems requires comprehensive analyses of relations between decisions and the consequences resulting from their implementations.

This paper discusses how heterogeneous knowledge coming from diverse fields of science and practice can be effectively exploited to develop mathematical models. In particular, selected problems related to integration of heterogeneous knowledge through interdisciplinary collaborative work are discussed; such work is performed by virtual modeling laboratories which are a combination of two concepts: (1) modeling laboratory (which comes from the concept of G. Dantzig, who stressed that models should be considered as representations of laboratory world), and (2) virtual organizations.

Next, the requirements for the modeling process supporting decision-making process are summarized. Then the structured modeling technology is outlined and it is explained how this technology responds to the summarized requirements. Finally, opportunities of exploiting models for knowledge creation are discussed.

Keywords: knowledge creation and integration, model-based decision-making support, virtual laboratories, knowledge civilization, structured modeling.

1. INTRODUCTION

Everybody solves many diverse problems and makes corresponding decisions everyday. Most of these processes are rule-based or even performed subconsciously. However, rational solving of many other problems requires a thorough analysis, which is conventionally called the decision making process. Complex problems cannot be rationally solved by intuition or experience supported by relatively simple calculations. Even the types of problems that used to be easy to define and solve have become complex because of the globalization of the economy, and a much greater awareness of its linkages with various environmental, social and political issues.

Rational decision making requires a comprehensive analysis of the underlying problem. Comprehensive analysis implies exploitation of pertinent science, i.e. organized knowledge relevant to the decision problem. Thus, knowledge should be a basis for rational decision making. This is commonly agreed but the consequences of this fact are not adequately understood.

For many complex problems a large part of pertinent knowledge can be represented by mathematical models. Model development requires collaboration of scientists and professionals who contribute (typically interdisciplinary and heterogeneous) knowledge. Such a collaboration is organized through virtual organizations, which for collaborative modeling can be called virtual modeling laboratories. In the final step of model development knowledge is created by model analysis, and used for supporting rational decision-making.

Thus this paper focuses on model-based support for solving complex problems, and is organized according to the above outlined process of knowledge integration and creation in virtual modeling laboratories. Section 2 discusses model-based knowledge integration, which is followed by a summary of key issues of collaborative modeling in Section 3. Structured Modeling Technology (SMT) is characterized in Section 4. The concepts of virtual organizations and of laboratory world are summarized in Sections 5 and 6, respectively. Section 7 deals with issues of knowledge creation through various elements of modeling process. Finally, Section 8 concludes the paper by summarizing main issues and outlining some open research challenges.

2. KNOWLEDGE INTEGRATION

Knowledge is typically understood as familiarity, awareness, or understanding gained through experience or study. The amount of knowledge is growing very quickly, therefore even best scholars can master only a tiny fraction of knowledge available in their professional area. Consider, e.g. mathematical programming, which is on the one hand a rather specialized area of mathematics, but on the other hand it is a rather broad area from the point of view of researchers working in a particular field (e.g. interior point methods for optimization, or wavelet-based approaches to analysis of time series).

Knowledge creation and integration is a rather complex process, which requires careful management, see e.g., [1, 2]. In this paper we focus on two specific issues: (1) knowledge integration for the development of mathematical models (discussed in this Section), and (2) knowledge creation by model analysis (in Section 7).

A common form of knowledge is a collection of facts and rules about a subject. Consider as an example a very simple subject, a cup of coffee. Very diversified knowledge is suitable for studying various aspects, e.g., how something (sugar, cream) is dissolved in the cup's content, or under what conditions the cup might break from thermal stresses, or what shape of cup is most suitable for use in aircraft, or how a cup of coffee enhances different people's productivity. An attempt to deal with all these aspects at once, and to represent all the accumulated knowledge pertinent to even such a simple topic would not be rational. Therefore, analysis of a problem, even when simple, typically exploits only a small fraction of the accumulated knowledge about the subject.

Complex problems are typically composed of heterogeneous subjects. For example, analysis of cost-effective measures of continental air pollution control aimed at improving environment quality, see the description of the RAINS model e.g., in [3], involves the following subjects: several sectors of economy (industry, transportation, agriculture, etc), technology, atmospheric chemistry, ecology, health, operational research, negotiations, policy making. Each of these subjects is rather complex, and for each there exist huge amount of knowledge accumulated in various fields of science and practice.

Although heterogeneity of subjects represented by the RAINS model is far beyond a typical complex model, selection of appropriate (for the problem at hand) elements of knowledge remains a challenge also for rather homogeneous (in terms of the science disciplines) problems.

Thus the first challenge in science-based support for solving complex problems is typically not the lack of knowledge but the selection of appropriate (usually tiny) fractions of knowledge from all relevant areas of science and practice. The second challenge is a reliable integration of the selected (typically heterogeneous) knowledge into a form in which it can be effectively used.

2.1. Requirement analysis

Actually, the two challenges summarized above are not addressed by a sequential process, they are typically solved in an iterative way driven by requirement analysis of the model-based support for solving the problem at hand. The role of requirement analysis is often underestimated although it is commonly known that a properly done analysis is a key condition for any successful modeling process. This topic is far beyond the scope of this

paper therefore we mention here only those key elements of the requirement analysis which are directly related to the process of knowledge integration and creation:

- what decisions are to be made,
- how the consequences of decisions are measured,
- what relations between the consequences and the decisions should be considered,
- what data is available,
- how user preferences (for different decisions and the corresponding consequences) can be represented.

Mathematical models are probably the best way to integrate knowledge for problem solving whenever it involves analysis of large amounts of data and/or not-trivial relations. In such cases the elements of the requirement analysis correspond to the basic elements of a typical structure (illustrated in Fig. 1) when using a mathematical model for problem solving.

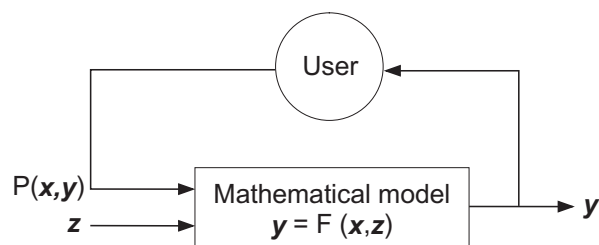


Figure 1: A typical structure when using a mathematical model for problem solving.

A mathematical model describes the modeled problem by means of variables, which are abstract representations of these elements of the problem, which need to be considered for the evaluation of the consequences (measured by outcome variables y) of implementing a decision (typically represented by a vector composed of many variables). More precisely, such a model is typically developed using the following concepts:

- decisions (controls, inputs to the decision making process) x , which are controlled by the user;
- external decisions (inputs) z , which are not controlled by the user;
- outcomes (outputs) y , used for measuring the consequences of implementation of decisions;
- relations between decisions x and z , and outcomes y ; such relations are typically presented in the form:

$$y = F(x, z), \quad (1)$$

where $F(\cdot)$ is a vector of functions (conventionally called constraints);

- a representation of a preferential structure $P(x, y)$ of the user, used for selecting (out of typically an infinite number of solutions) a manageable subset of solutions correspond best to user's preferences.

The compact form of (1) does not illustrate the complexity of the underlying knowledge representation: a large model may have several millions of variables and constraints, even when the number of decision and outcome variables is much smaller (say, several thousands).

2.2. Knowledge integration in models

In order to outline the knowledge integration let us consider a mathematical model as composed of entities and relations between them. Entities are of two types: (1) parameters, values of which represent pertinent information (i.e. a collection of data), and (2) variables, values of which are assigned during the model analysis. The model relations (conventionally called constraints or functions) represent knowledge about the relationships among the model entities.

A model therefore integrates knowledge pertinent to solving a particular problem on two levels:

- symbolic model specification,
- model instance (called also *substantive model* or *core model*) composed of model specification and a selected set of data used for instantiation of relations (through assigning values to parameters of the relations),

In many situations symbolic model specification can be based on commonly known rules of science. However, in other situations knowledge pertinent to a particular relation is so diversified that a definition of the relation requires a dedicated study. To illustrate this problem let us recall that the relation between tropospheric ozone and its two precursors (nitrogen oxides and volatile organic compound) can be defined in very different ways, each having the corresponding diversified advantages and disadvantages depending on the content in which the relation is applied (see e.g., [4]).

For large scale models relations for each subject (represented by a submodel) are defined in a close cooperation between specialists in the corresponding area and a team of modelers capable to:

- assess the consequences of the considered relation types on numerical complexity of the resulting computational tasks,
- assure consistency of the whole model to which the relation will be included.

Thus the development of symbolic model specification requires:

- analysis of a relevant (for the purpose of the model) knowledge about each modeled subject (submodel), and a selection of these elements of the knowledge which will be represented in the model,
- representation of the selected knowledge in a mathematical form consistent with relations defined for all other submodels,
- integration of all submodels into a consistent model

that possibly best (in terms of both required accuracy and computational efficiency) represent the relations between the decisions and outcomes.

We should stress an important feature of a properly developed model: it integrates knowledge in a reliable way thus provides an objective and justifiable way of analyzing the relations between the decisions and the consequences of their implementation. This objectivity can be assured only if:

- all model relations are actually based on knowledge, i.e. on verifiable facts and rules;
- the assumptions for these facts and rules are consistent with the assumptions agreed for the model;
- semantic correctness is enforced not only for each relation but also for the set of all relations (e.g., the units and the accuracy/precision of all entities are consistent);
- no representation of the preferential structure is included in the substantive model;
- data used for model instantiation is consistent with the model specification.

A more detailed discussion on development of models for decision making support is available e.g., in [5, 6], and a general presentation of knowledge integration and creation on knowledge Web is available in [7].

Although a proper symbolic model specification is certainly the most challenging part of model building from the knowledge integration point of view, we have to stress that the data used for model instantiation also represents a necessary part of knowledge which needs to be integrated into the modeling process in a robust and efficient way. We comment on this issue in Section 3.2.

3. COLLABORATIVE MODELING

Mathematical modeling of a complex problem is actually a network of activities involving interdisciplinary teams collaborating closely with experts in modeling methods and tools. Dantzig summarized in [8] the opportunities and limitations of using large-scale models for policy making. Thanks to the development of algorithms and computing power today's large-scale models are at least 1000-times larger; thus, large-scale models of the 1970s are classified as rather small today. This, however, makes the Dantzig's message relevant to practically all models used today, not only for policy-making but also in science and management.

Today's models are not only much larger, but the modeled problems are more complex (e.g., by including representation of knowledge coming from various fields of science and technology), and many models are developed by interdisciplinary teams. Moreover, the modeling processes supporting policy making have to meet strict requirements of: credibility, transparency, replica-

bility of results, integrated model analysis, controllability (modification of model specification and data, and various views on, and interactive analysis of, results), quality assurance, documentation, controllable sharing of modeling resources through the Internet, and efficient use of resources on computational Grids.

Traditional approach to modeling is based on the assumption that a small team can organize and document a modeling process. However, this approach is neither reliable nor efficient for complex models developed by several (or more) teams working intensively¹ at distant locations. To illustrate this statement let us characterize collaborative work for the selected stages of modeling process discussed below.

3.1. Model specification

As discussed in Section 2, model specification is composed of specifications of submodels (built for distinct subjects), and each submodel requires selection of pertinent knowledge and its mathematical representation. Thus each submodel is typically developed and tested by a small team composed of specialists in the modeled subject and at least one specialist in mathematical modeling. Provided that the requirements for knowledge integration summarized in Section 2 are met, the submodels can be gradually (i.e., not all submodels are combined at the same time) integrated in the whole model.

A representation of the model specification should:

- allow to use a single source for all remaining elements of the modeling process (creation of model instances, generation of computational tasks, interpretation of results, and documentation);
- provide meta-data necessary for:
 - ★ creating data structures for all model parameters;
 - ★ semantic check of data correctness; and
 - ★ creating data structures for results of various analysis.

These requirements are implied by heterogeneity and size of complex models, which in turn call for participation in the modeling process of many persons with diversified backgrounds playing different roles at various stages of model development.

It is the qualitative increase of model size and heterogeneity that requires different (from the traditional) way of collaborative modeling. This impact is illustrated in the discussion of data handling problems.

3.2. Data

Data maintenance for a large complex model is by far the most risky element of any modeling process. The popular saying “*garbage in, garbage out*” for large amounts

¹This implies that diversified elements of the model are developed/modified practically at random times.

of data implies that incorrectness of even a tiny fraction of all data may lead to very misleading results from the model analysis. The problem may be difficult to trace because, for some analyses, even “very wrong” data elements may not have any practical impact on the corresponding solutions (even if a sensitivity analysis would indicate it should), while in other situations even a relatively small mistake may result in a dramatic difference between two sets of solutions (for wrong, and correct data, respectively). Collecting and verifying data needed for a small model is a relatively simple process as compared to data management of large models. To illustrate this let us assume that one needs only one minute to collect and verify one data item (which is certainly an underestimation). A typical model used in text books has fewer than 20 elements of the Jacobian, therefore its data can be collected in less than an hour and can be presented in a fraction of a page (either printed or displayed) for relatively easy verification. However, the Jacobian of the new version of the RAINS model will have over 10^{11} elements. Therefore assuming a working year composed of 1800 hours, collection and verification of 10^{11} data elements would require about 10^6 person-years. Fortunately, large models have sparse Jacobian, but human resources needed for collection and verification of nonzero elements still amounts to a large number of person-years.

Data for large models comes from different sources (also as results from analysis of various models), and larger subsets of data are maintained by teams. Fortunately, there is a natural division of data into subsets, which are maintained by individual persons or small teams. Persons working with well-defined subsets of data are experienced in collecting, cleansing, verifying, and maintaining the data they are responsible for. Therefore the “only” problem is how to structure the process of aggregating the subsets of data maintained by various teams (typically also using different hardware and software) into a data collection that can be used for model instantiation and analysis. To achieve this, a structured approach based on DBMSs is a must.

3.3. Model analysis

Knowledge about the modeled problem is actually created by model analysis. This topic is discussed in Section 7.

4. MODELING TECHNOLOGY

The complexity of problems, and the corresponding modeling process are precisely the two main factors that determine requirements for modeling technology that substantially differs from the technologies successfully applied for modeling well-structured and relatively simple

problems. In most publications that deal with modeling, small problems are used as an illustration of the presented modeling methods and tools. Often, they can also be applied to large problems. However, as discussed above, the complexity is characterized not primarily by the size, but rather by: the requirements of integrating heterogeneous knowledge, the structure of the problem, and the requirements for the corresponding modeling process. Moreover, efficient solving of complex problems requires the use of a variety of models and modeling tools; this in turn will require even more reliable, re-usable, and shareable modeling resources (models, data, modeling tools). The complexity, size, model development process, and the requirements for integrated model analysis form main arguments justifying the needs for the new modeling methodology.

Structured Modeling Technology (SMT) described in [3] has been developed for meeting such requirements. SMT supports distributed modeling activities for models with a complex structure using large amounts of diversified data, possibly from different sources. A description of SMT is beyond the scope of this paper, therefore we only summarize here its main features:

- SMT is Web-based, thus supporting *any-where, any-time* collaborative modeling.
- It follows the principles of Structured Modeling proposed by Geoffrion, see e.g., [9]; thus it has a modular structure supporting developments of various elements of the modeling process (model specification, (subset of) data, model analysis) by different teams.
- It provides automatic documentation of all modeling activities.
- It uses a DBMS for all persistent elements of modeling process, which results in efficiency and robustness; moreover, the capabilities of DBMSs serve efficient handling of also huge amounts of data.
- It assures the consistency of: model specification, metadata, data, model instances, computational tasks, and results of model analysis.
- It automatically generates a Data Warehouse with efficient (also for large amounts of data) structure for:
 - ★ data, and tree-structure of data updates,
 - ★ definitions of instances,
 - ★ definitions of preferences for diversified methods of model analysis,
 - ★ results of model results,
 - ★ logs of all operations during modeling process.
 This conforms to the requirement for persistency of all elements of modeling process.
- It exploits computational grids for large amounts of calculations.
- It also provides users with easy and context sensitive problem reporting.

More detailed arguments (including overview of the standard modeling methods and tools) supporting this statement are available in [3].

5. VIRTUAL ORGANIZATIONS

The fast development of the Internet calls for its more advanced use, i.e. for jumping from passive access to distributed information to collaborative integration and creation of knowledge contained in models. This requires dynamic management of interdisciplinary teams contributing the needed disciplinary knowledge (typically available at different organizations).

A more advanced use of the Internet has been recommended already in [10]. The concept of *Virtual Organization (VO)* in the context of the Grid is presented in [11] together with basic characteristics of VOs (such as authentication, authorization, resource access, resource discovery) that are also typical for collaborative modeling activities. A vision of a semantic grid for future e-science infrastructure in a service-oriented view is discussed in [12]. It is built around knowledge services, which support management and application of scientific knowledge in order to respond to growing needs of collaboration between large scientific teams.

Unfortunately, the modeling community is far behind other scientific communities, which exploit the Internet capabilities for Computer Supported Collaborative Work (CSCW) more efficiently. One of the most advanced and innovative developments in CSCW are the so-called *collaboratories*.² The dramatic increase of the power of diversified communication and computational technologies during the last two decades has resulted in the creation of thousands of virtual laboratories, which facilitate the long-distance CSCW of multidisciplinary teams, often using complex instrumentation in real-time mode. Collaboratories are a rather small subset of virtual laboratories that are organized as a problem specific, hand-crafted projects supporting three types of communications: (1) people-to-people communication, (2) long-distance real-time control of complex instrumentation, and (3) remote access to information. The reliability and efficiency requirements of the second element call for exploiting the most advanced technology for collaboratories.

The need to exploit rich resources of knowledge for model-based decision support is widely recognized. Solutions to various elements needed to achieve this have been discussed in e.g., [13, 14, 15]. However, these partial solutions have never been used to provide an inte-

²The term "collaboratory" was coined in 1989 by W. Wulf to refer to the use of diversified technologies available for long-distance collaboration, see e.g., <http://www.scienceofcollaboratories.org>.

grated and comprehensive modeling environment to efficiently utilize the resources available on the Internet. Thus, despite the unquestionable progress in the modeling and Grid technologies, there is still a lot of work to be done in exploiting available technology, knowledge and experience.

6. LABORATORY WORLD

The requirements of complex problem modeling demand a qualitative jump in modeling methodology: from supporting individual modeling paradigms to supporting a *Laboratory World*³ in which various models are developed and used to learn about the modeled problem in a comprehensive way. The truth is that there are no simple solutions for complex problems. Thus, learning about complex problems by modeling is in fact more important than finding an “*optimal*” solution.

Laboratory World requires integration of various established methods with new (either to be developed to properly address new challenges, or not yet supported by any standard modeling environment) approaches needed for appropriate (in respect to the decision-making process, and available data) mathematical representation of the problem and ways of its diversified analyses. Therefore, to be able to adequately meet the demand for advanced modeling support one indeed needs to develop and apply novel modeling methodologies.

Such a laboratory world is actually supported by the SMT outlined in Section 4. SMT is being gradually enhanced to fully meet the following requirements:

1. The demand for integrated model analysis, which should combine different methods of model analysis for supporting a comprehensive examination of the underlying problem and its alternative solutions.
2. Stricter requirements for the whole modeling process, including quality assurance, replicability of results of diversified analyses, and automatic documentation of modeling activities.
3. The requirement of controlled access through the Internet to modeling resources (composed of model specifications, data, documented results of model analysis, and modeling tools).
4. The demand for large computing resources (e.g. large number of computational tasks, or large-scale optimization problems, or large amounts of data).

7. KNOWLEDGE CREATION

Diversified knowledge is created during model-based problem-solving processes. Such knowledge is either

tacit (thus, usually not documented) or explicit. We outline in this Section the main processes contributing to knowledge creation.

7.1. Model development and analysis

In fact, the primary goal of modeling is to create knowledge about the modeled problem. Actually, model-based learning about the problem is typically even more important than finding *the best* solution, see e.g., [6]. Thus, a huge amount of knowledge has been created by various types of analyses of a countless number of models. Unfortunately, this knowledge is often difficult to use beyond the modeling process. The main reason for it is insufficient semantic description of model results. These are typically consumed for the analysis of the decision problem at hand, and not documented sufficiently for reuse in different contents.

We should stress that a truly integrated model analysis should exploit diversified paradigms of model analysis, see e.g., [6]. Moreover, some problems require rather specific methods of model analysis, see e.g., [4, 16].

A lot of knowledge has been created during various modeling activities in response to the needs that could not be met by then available methods. In fact knowledge had to be created for each topic discussed in Section 2 before it was integrated into a modeling process.

Thus there is a cycle of knowledge creation, integration with other knowledge for various modeling activities, and subsequent creation of new knowledge in response to the recognized limitations of the available knowledge.

7.2. Model-based problem solving

A lot of knowledge has been created while coping with limitations of existing methods serving model-based support for problem solving. Many break-through developments have been necessary to move from the traditional OR (Operations Research) approach to a diversified set of methods and tools available today for decision-making support for problems of different types to be solved by DMs with different habitual domains.⁴ As examples of this type of knowledge we mention four methodologies:

- Shinayakana system approach, see e.g., [18, 19]. Shinayakana methodology is based on Japanese intellectual tradition, which takes into account limitations of our abilities to understand and analyze problems, and provides constructive methods for model-based problem solving.

⁴A fairly stable set of ways of thinking, evaluating, judging and making decisions. Yu [17] presents all aspects of habitual domains: their foundations, expansions, dynamics and applications to various important problems in people’s lives, including effective decision making. The concept of habitual domain is based on an integration of psychology, system science, management, common sense, and wisdom.

³Originally proposed by Dantzig, see e.g. [8].

- *i*-System, see e.g., [20, 21], is a systems methodology composed of five subsystems: scientific approach, information science, social sciences, knowledge science, and systems science used to manage these four different but complementary approaches.
- Meta-synthesis approach, see e.g., [22]. The essential idea of this approach is to unite an expert group, all sorts of information, computing technology, as well as interdisciplinary knowledge for proposing and validating hypothesis.
- Model-based decision support. One of several European approaches to develop analytical models, and apply multicriteria model analysis (which includes traditional simulation and single-criterion optimization) for effective decision-making support is presented in [5]. The approach combines knowledge from technical fields (control theory, optimization) with concepts of knowledge in humanities and social sciences, and with lessons from actual applications of model-based support for decision-making.

Actually, all four methodologies have more in common than can be seen from this short summary. This is yet another example of knowledge integration, which has resulted from long-term contacts between scientists originally coming from very different cultures and scientific schools.

7.3. Modeling technology

SMT has been developed in response to the modeling needs of the RAINS model, which could not be met by the available modeling tools. Although SMT exploits a great deal of modeling legacy, a number of challenging problems had to be solved to provide the needed functionality. This includes the SMT features summarized in Section 4.

7.4. Computational tasks

Sometimes a simple modification of a model specification results in a dramatic decrease of the computing resources needed to solve the underlying computational task, or in providing a stable solution, or even makes it possible to solve the optimization task. Several examples illustrating this point can be found in [7].

8. VIRTUAL MODELING LABORATORIES

Mathematical modeling has been playing an important role in knowledge integration (during the model development) and creation (primarily during model analysis). However, there are still many possibilities for a qualitative improvement of knowledge management during the modeling process, see e.g., [23]. To achieve this one

needs to exploit the synergy of three fields: advanced modeling methods, knowledge science, and modern networking technology.

Thousands of organizations worldwide develop and work with models. These models store huge amounts of knowledge and expertise. Models integrate knowledge in two forms: analytical relations between entities (parameters and variables) used to represent the modeled problem, and data used for defining parameters of these relations. Models are typically also used for creating knowledge about the modeled problem: not only by knowledge discovery methods using data provided by various model analyses, but also during the model verification and testing. Moreover, modeling knowledge is also often enhanced while coping with development and analysis of complex models.

This paper presents opportunities of combining the results of recent developments in knowledge science with capabilities of structured modeling, and of modern computing technology in order to efficiently support knowledge integration and creation by collaborations of interdisciplinary teams working in distant locations.

In addition to the challenges discussed in this paper we should stress the importance of a proper treatment of uncertainty. This topic is far beyond the scope of this paper, thus we can only suggest to consult [24, 25] for a summary of experience and open research problems related to effective treatment of endogenous uncertainty for supporting policy making.

We conclude with an obvious observation: complex problems can be solved only if data, knowledge, and information are not only available, but can be efficiently analyzed and shared, which in turn requires mathematical modeling; this typically requires reliable integration of knowledge from various areas of science and practice. This paper shows that meeting the resulting requirements calls for a closer collaboration of researchers working in various fields, but especially in knowledge science, operational research, mathematics, and control. Experience has shown that interdisciplinary approach to addressing challenging problems has often produced qualitative improvements in solving complex problems.

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