Lie Algebraic Methods as Mathematical Models for High Performance Computing Using the Multi-agent Approach

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Abstract. In this paper we discuss some problems of the construction of mathematical models of dynamic processes to effectively carry out computational experiments using high performance computing systems (both parallel and distributed). The suggested approach is based on the Lie algebraic approach and the multi-agents paradigm. The Lie algebraic tools demonstrated high effectiveness in dynamical systems modeling. A matrix presentation for dynamical systems propagation allows to implement a modular representation of the objects of study as well as the corresponding operations. Moreover, the matrix formalism is based upon the multi-agent paradigm for modeling and control of complex systems for physical facilities. The corresponding codes are realized both in symbolic and numerical forms.

1 Introduction

In today's world the role of experimental physics is growing on one hand as a source of new knowledge in the various fields of science and technologies (not only in high-energy physics), and on the other – as a field of knowledge, in which new methods and tools for modeling complex processes of different nature are constantly generated. In this case under the complexity of the modeling process and the complexity of the governance structure we understand not only a huge number of control actions, but also the complexity of behavior of management subjects. Moreover, in physics of particle beams, plasma physics, and a number of other areas there is a three-tier control structure. The object of control is beam (ensemble) of particles and the subjects of the first level are presented by control mechanisms consisting of control units that provide the necessary (optimum) conditions for the evolution of the particle beam. Finally, second level control subjects are presented using information elements of the system which controls (based on certain principles) enormous number of control devices (magnets, multipole lenses, etc., diagnostic systems for plasma, beam etc.), see, for example, [1]. In particular, a common problem in the cyclic accelerators is the necessity for careful monitoring of certain characteristics of the particle beam for a long period of time with minimal loss of intensity of the beam, while ensuring the necessary degree of stability of the particle beam parameters and so

O. Gervasi et al. (Eds.): ICCSA 2016, Part I, LNCS 9786, pp. 418–430, 2016.
DOI: 10.1007/978-3-319-42085-1_32

on [2]. Unlike mechanical systems, in this class of problems we are dealing with complex behavior of the ensemble of particles (both regular and chaotic) that is in need of special mathematical tools, taking into account the collective nature of the beam (control subject). Regarding the controls (first level entities), they are usually realized with the aid of electromagnetic fields, which are distributed in space). The difficulty of formalization and management at this level is related to the spatial distribution of the control field, and is caused by the limited knowledge not only about the state of the ensemble of particles, but also about "field configurations". This knowledge restriction is determined mainly by some limitations in hardware installation of control elements and other factors which affect the quality control.

Taking into account the problems mentioned above, in this paper we consider a three-tier computing scheme: a physical object – a mathematical model – an information model. In other words, we can say that the distributed nature of a control object (particle beam) and control subject (in our case the electromagnetic field) leads to the necessity of building distributed information environment adequate for such physical features. Using technologies of multi-agent systems maximizes adequacy of the process of mapping of the physical model onto the relevant information model. Implementation of necessary computational experiments is carried out using parallel systems (for example, GPU-Accelerated Research Clusters) and distributed computing. It should be noted, that after construction of relevant information units we should incorporate this triune structure into the concept of the Virtual Accelerator, see, e. g. [3].

2 A Multi-agent Concept

The above mentioned reasons lead to the necessity of forming a management information system (the phase of control subject of the second level). This system has to provide the necessary tools for adaptation of electrophysical devices of standard control systems using a multiplicity of control parameters, as well as multiplicity devices that provide necessary information about the state of the control object – the particle beam. We should note that this hierarchy can also be used for modeling systems of control in biological systems, economics and other distributed (in time and space) systems. In other words, our goal is to create an information control system that is based on the rather limited amount of experimental data and can offer a variety of scenarios for implementation of "optimal" regimes of systems functioning.

In some papers published previously by the author the concept of Lego-objects was proposed (see, e. g., [5,6]), which operate as independent and specialized control objects, implemented in the form of special computer programs (including methods and technologies of artificial intelligence). The realization of similar concept is largely determined not only by the structure of subject and object management, but also by the methods used for mathematical models construction. The corresponding mathematical models should be adequate both to a description of physical problems, and to the corresponding operations in computational environment.

Indeed, the introduction of Lego-objects allows us to allocate relevant knowledge and resources among sufficiently "independent" intelligent objects (according to modern terminology – agents) for distributing rights in control procedures in whole, and also for process of problem-solving and for ensuring the implementation of some specified modes (an optimal in some sense).

At the same time, we reserve a narrow functional orientation of our agent (a Lego-object) on a separate part for the overall solution of the problem. However, the totality of similar agents, considered as a single system, gradually began to give way to universal integrity (autonomy of the control system as a whole). In other words, according to the concept of multi-agent technology (see [7]), for solution of this controversy we suggest a new method for control problems in complex physical systems.

In other words, we offer a decentralized system (in contrast to classical centralized control system), in which the control procedures are realized at the expense of local interactions between agents. At the same time, we should preserve functional orientation of our agent (a Lego-object) on a separate part of the overall solution of the problem narrow enough. However, the universality of such agents gradually begin to give way to universal integrity of an informational system as a whole. It should be noted, however, that incomplete universality of individual agents are caused by large variability of practical oriented tasks that need to be addressed in accelerator physics problems.

Usually, in the classical approach we use a set of well-defined algorithms which can help to find the best solution for the control systems of ensembles of particles (in accelerators, thermonuclear facilities – tokamaks, stellarator, etc.). But the complexity of the control systems for similar systems incites us to change of paradigm of control both in theoretical and practical aspects. The multi-agent paradigm can also decrease both the computational burden and the corresponding computational time. This also motivates us to the need for a concept of complex physical processes management using the intellectualization of the user interface.

Common understanding of the properties of the agent requires formulation of some criteria of optimality. The agent has the ability to interact with the environment. Thus, the agent is an entity that is installed in an external environment and can interact with it. This agent can and should make a decision for autonomous rational action to achieve defined goals. Under the intelligent agent we understand an entity featuring the following properties:

– *reactivity* – the agent perceives the environment and reacts to changes in it, performing actions to achieve the goals specified;
– *proactivity* – showing an agent behavior goals, showing initiative to commit actions aimed at achieving the given objectives;
– *sociality* – the agent interacts with other entities of the environment (first of all with other agents) to achieve formalized objectives.

Implementation of the first two properties separately can be achieved quite easily. However, trying to combine these two properties in a system (in specified proportions) researchers typically face a number of difficulties. Indeed, the operation of the agent is not effective enough both in the case of a rigid script execution for achieving the goal (in other words, ignoring the changes in the external environment) and in the absence of the ability to notice the need to adjust the plan. Here we can note that it is the result of inefficient work in response only to environmental stimulus neglecting the planning of targeted actions.

Implementing the third property can be a difficult problem, because here we can usually surmise not only communication with each other, but also certain elements of the "cooperation" with other entities of control process. In other words, it is necessary to provide separation between the objectives of specific agents and joint planning and coordination of actions aimed at achieving common goals. So, a "social behavior" requires from the agent the corresponding representations not only about goals of other agents but also about how they design scripts to achieve these goals. The analysis of control systems for complex physical processes leads us to the conclusion about the lack of a priori precision for all conditions of operation. This leads us to necessity of description of adaptive formalization of investigated problems, having such an attribute of the agent as adaptability, i. e. the ability to automatically adapt to uncertain and changing conditions in a dynamic environment. The agent operates in a complex, changing environment, interacting with other agents. This leads to the fact that the multiagent system is much more effective in comparison with a "standard" adaptive system, since similar system can be trained faster for operating more efficiently due to redistribution of functions and/or tasks between agents. The notion of complex systems is linked with the following fundamental ideas that directly affect the functioning multi-agent systems. We list these ideas ([7], for example) below:

- in complex systems there exist autonomous objects that interact with each other in carrying out their defined tasks;
- agents must be able to respond to changing conditions in the environment, in which they operate, and possibly change its behavior on the basis of the information received;
- complex systems, which are characterized in terms of emerging (temporary and/or permanent) structures, and are logically represented by schemes which are formed by the interaction between the agents;
- complex systems with emerging structures often oscillate between order and chaos;
- biological analogies (such as parasitism, symbiosis, reproduction, genetics, mitosis and natural selection) are often used when creating complex agent-based systems.

The concept of agents developed in the framework of multi-agent technology and multi-agent systems, automatically implies an active behavior of the agent, in other words the ability of the computer program itself to respond to external events and "choose" the appropriate actions. In view of the above, in the future we will stick to the following definition of an agent.

Definition 1. *An agent is a certain software unit capable of acting for the purpose of achieving the goals set by the user.*

Thus, returning to the concept of Lego-objects in view of the corresponding definitions, it can be argued that the Lego-object has dual nature. First – from mathematical point of view it describes the subject area (in our case, the ensembles of particles, electromagnetic fields, etc.). It's second "essence" (informational) presents the interaction of these objects in the process of computational experiments and in the process of creating a scenario for control of the behavior of the beam by using control devices (or rather, using electromagnetic fields generated by these devices). We should note that in modern literature devoted to accelerator physics the concept of the Virtual Accelerator is being actively discussed (see [3]).

In almost all publications quite traditional modeling and control systems are considered despite the ever-increasing requirements for physical experiments support.

However, the approaches developed in these articles are quite different. We can conclude that a plurality of characteristics of control devices of the particle beam on one hand, and complexity of strict optimality formalization, on the other hand, leads us to the need of using methods of multi-agent approach. In other words, we need to introduce a family of independent "executive agents" with different functionalities (with different specializations), that interact with each other in accordance with prescribed rules: synchronizing actions, exchange of information, automated adaptation to uncertain and variable conditions of the dynamic medium etc.

3 Classes and Subclasses of the Lego-Objects

Following the previously proposed concept of Lego-objects, we describe the hierarchical structure of mathematical objects that are used to build mathematical models of physical processes occurring in the accelerator facilities. We should note that many objects can also be used in other problems of computational physics, which are described in terms of nonlinear dynamical systems. We should note that the idea of multi-agent systems is actively implemented in many systems of mathematical modeling (see, for example, the package Mathematica [8]), indicating the relevance and effectiveness of this approach for a wide class of problems. So, following the concept described above, we have a three-tier structure of control: the control object (an ensemble of particles) – a system of control (the subjects of the first level) – the subject of the second level – an informational system, which realizes the control strategy. We should note that one of the most important principles to be followed is the universality of information units "gluing" at all levels, thus ensuring the universality and interoperability in terms of preserving the information structure. In this case, we mean the fact that the properties of a computational model for each information unit at all stages of the simulation should lead to the correct result in terms of performing computations of corresponding mathematical operations for solution of our practical problems.

In case of the evolution of particle beams in accelerators (or plasma particles in the corresponding systems), dynamics of the particles is described by nonlinear systems of motion equations. Furthermore, it is often necessary to take into account additional factors (e. g. effect of beam polarization, interparticle interaction and etc.). Note that each of said blocks can have different shapes which correspond to physical description of an object and can be processed according to the chosen model of computational process. If we can provide researchers with a sufficiently extensive set of facilities and operations at any stage of modeling, then researchers can replace corresponding modules (after comparing respective results with empirical ones) and thereby formulate certain additional conditions for an optimal dynamic regime or for the target result. In accordance with the concept of Lego-objects, we can modify necessary information items for execution of corresponding computational experiments. In other words, these information items describe the nature of intelligent agents, which are supplied with special attributes. Moreover they can be considered as meta-objects that can affect other objects, as well as possess a necessary set of instruments developed for interaction with the environment and other meta-objects.

3.1 Construction of Information Units

As shown in [4], the main type of agents from a mathematical point of view is a matrix with certain matching rules, which leads to the correct description of the beam evolution in the accelerator facility. At the same time, all the characteristics of the particle beam (control object) and external field (control sub-object) can also be expressed using the matrix representation, and the corresponding mathematical operations. Here we should mention such matrix operations as Kronecker sums and products. There is also a set of permitted associations of subagents, which is determined by the physical nature of the respective objects. Here is the view of the rules that define the necessary properties of the original physical object, and on the other – the rules by which the appropriate agent or subagent interacts with other agents (subagents) for optimal results. In this section, as an example, we consider the structure of the description of a controlling agent responsible for some physical element. In our example, we consider a magnetic or electric quadrupole as a control element. As mentioned above, the corresponding agent (possessing an integrity property from physical standpoint) from a mathematical point of view can be represented as a compound information essence, which is considered as a set of subagents that are not self-sufficient by themselves, but determine the integrity of the agent in whole (see Fig. 1).

The physical parameters that define configuration of the field on each interval and are included in the matrix $\mathbb{M}^{1k}$ represent information units, which are responsible for the appropriate subagents. Thus, we formulated the physical nature of the problem being solved in terms of information objects. In addition, we have to impose certain rules on the choice of necessary parameters and put

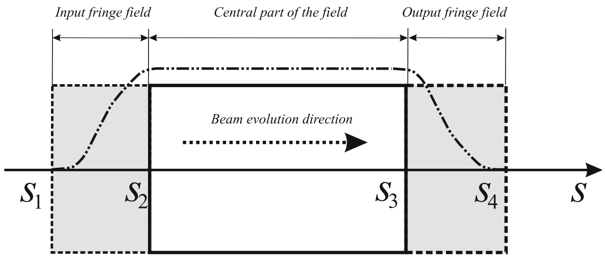

Fig. 1. The scheme of the modeling process interpretation.

them in our set of determining rules for “assembly” of subagents in a single agent, and thereby provide a physical meaning for all “aggregate” agents. The complete set of similar components should be classified by their physical interpretation, as well as their significance. This allows you to build a hierarchy of proper relations for corresponding interactions of all agents for solution of the investigated problem.

Thus, subagents which are responsible for the fringing fields can be used for describing possible configurations of fringe fields (satisfying to the Laplace equation). The corresponding admissible set of fringe fields should be determined using both experimental data and theoretical investigations, see, for example [5,9]. Accordingly, all components of the control field (the central part of the field, contribution of fringe fields – input and output parts) in a general field up to the N-order should be taken into account. This leads to the fact that the matrix for the total field is the product of the respective matrices. In other words, the matrix of the mapping for the total field of our quadrupole lens can be written up to the N-th order in the following form

$$\mathbb{M}^N(s_4|s_1) = \mathbb{M}^N(s_4|s_3)\mathbb{M}^N(s_3|s_2)\mathbb{M}^N(s_2|s_1) = \\ = \left\{\sum_{k=1}^{N}\mathbb{M}^{1k}(s_4|s_3)\right\}\left\{\sum_{k=1}^{N}\mathbb{M}^{1k}(s_3|s_2)\right\}\left\{\sum_{k=1}^{N}\mathbb{M}^{1k}(s_2|s_1)\right\}. \quad (1)$$

This multiplicative form allows us to calculate the total matrix as a product of partial matrices and can be constructed on all subintervals in according the rules described in [6] both in symbolic and numerical form. Necessary control over the quality of the computational procedures can be carried out using the methods set out in the articles [10,11].

In addition, we have to not only define special rules for the choice of these parameters, but also preserve them in the form of corresponding rules for forming of subagents as a single agent. On the next step we should provide a physically meaningful “cross-linking” of all agents for description of rules. The corresponding set of similar rules must have the necessary physical interpretation. This allows us not only to build a hierarchy of relations for corresponding interactions of all agents for solution of our problem, but also to automate the process of forming corresponding matrices.

Here is the view on the rules that on one hand define the necessary properties of an original physical object and on the other – the rules by which the appropriate agent or subagent interacts with other agents (subagents) for optimal results. In addition we have to impose certain rules for the choice of these parameters as well as to transform them in a complex of corresponding rules for concatenating of subagents into an integral whole. We should note that the corresponding family of rules consists of two subfamilies. The first contains prohibitive rules of cross-linking, while the second defines flexible adjustment of rules for cross-linking of sub-agents into a single agent. In the next step we need to formalize the physical cross linking rules for all agents. This is necessary to "physical users" for formal descriptions of informational units using the corresponding physical interpretation.

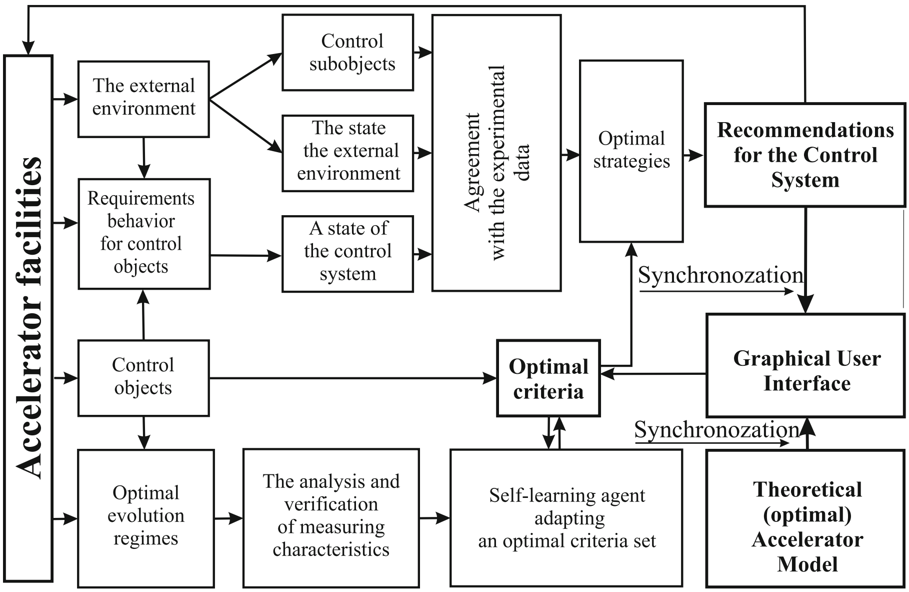

Fig. 2. The scheme of the modeling process interpretation.

So, the physical parameters that define the control field configuration on each interval and included in the matrix $\mathbb{M}^{1k}$ are incorporated as information parameters for appropriate ordered subagents. So the physical core of the problem of fringe fields can be interpreted in terms of some set of information objects. However, at first we have to impose certain rules for the choice of control parameters and then formulate the rules for corresponding "inclusion" of subagents into a single agent in according to chosen optimal strategy. So, we have reasonable physical restrictions for our agents and we have enough freedom to implement the search for optimal solutions. Naturally, the optimality criteria depend on the problem under consideration, but they can be clearly formalized in terms of the corresponding matrices $\mathbb{M}^{1k}$. It should be noted that this allows you to search the optimal regimes not only using various methods of parametric optimization, but also using the corresponding physically intuitive and experimental knowledge. It should be noted that in the first case specified parameters lose their physical content, which greatly simplifies the optimization process using multi-agent technology. Typically, similar problems can be solved within the different concepts of global optimization (e. g., [12]), but a large number of parameters and the complexity of computational procedures (and thus significant computational cost) lead to the need to use alternative methods for finding optimal solutions.

Here we must make an observation that in this class of problems (management of complex distributed systems) an optimization problem itself is formulated as the task of finding not only the optimal solution (in some sense), but the best solution possible (taking into account the formalized tasks in the experiment). This approach is adequate to meet the concept of the Virtual Accelerator. The point is that in large control systems for large physical facilities (accelerators, tokamaks, and etc.) the control is not carried out in an online mode (the speed of behavior of the physical processes is significantly higher than response speed of corresponding control systems). It should also be noted that the training session for a control system, based on the multi-agent technologies can be realized much easier if the requirements for stability of the system under small variations of control parameters are met. The fact is that this property of stability may be incorporated into the properties of the agents (subagents) naturally.

Moreover, since there exists a memory effect of intelligent agents, then if we have a set of "successful" combinations it allows to find appropriate solutions using the accumulated information (memory effect or adjustment of intelligent agents) for certain class of problems. We should also point out the need for a mechanism to monitor the correctness of all implementation procedures. The general scheme of interaction between logical blocks in the search for optimal solutions based on the matrix formalism for dynamical systems and multi-agent approach is shown on Fig. 2.

3.2 The Architecture of Classes and Subclasses of Agents

It is well known that a distributed multi-agent system may be divided into two classes: one class is composed of systems of "highly intelligent agents", while the second class is based on the so-called group mind. It should be noted that this classification corresponds to two classes of opposite options for multi-agent systems. The above concepts of agents and sub-agents allow us to consider the proposed multiagent system as a mixed class with the dynamic nature of the formation process for the implementation of such a system. Thus, the proposed variants are used for formation of classes of agents and sub-agents may be implemented in a dynamically generated computing environment. Indeed, the first class is suitable for implementation on distributed systems with a fairly small number of agents, while the second class uses a relatively small number of servers. In this case the agents themselves are not complicated objects and therefore can be implemented using simple algorithms for their interaction. Indeed as such agents act they introduce subagents. Moreover, it's principally possible to introduction a hierarchy of agents according to complexity and scope of the operations. This approach "fits in" well with the above ideology based on one hand on the matrix formalism, and on the other – on the concept of Lego-objects (see Fig. 3).

To implement the approach described above, we considered various techniques, in particular, for multi-agent systems construction a set of ready-to-use components Magenta Toolkit technology[1] has been considered. The proposed set of components Magenta Toolkit is a software tool (written in Java) that greatly simplifies and accelerates multiagent systems development for a variety of complex tasks. Knowledge which are inherent in our area of problems (beam physics and plasma) are notable for not only the large number of interconnections, but also for high computational complexity (which is usually absent in the "standard" problems). One should also consider the large number of many individual factors specific to various controls, as well as the nonlinearity of the corresponding evolutionary processes (nonlinear dynamics of particle beams).

In constructing the necessary software, for knowledge required for its functioning can be divided into the domain knowledge and the knowledge needed for the task and/or decision-making. In our case, the subject area comprises a mathematical model of corresponding physical reality and certain management rules (including the optimal), based on the matrix formalism for description of particles dynamics in the accelerators. On the second step we should include methods and tools for decision-making and description of relationships between agents. To describe the subject domain we can use the Domain Ontology, while for the implementation of methods for decision-making – the ontology of "virtual market" (Virtual Market Ontology), see [13]. Based on the above, appropriate ontologies can be represented in the form of the corresponding circuit of Fig. 3. It should be noted that one of the features of ontologies application is to use them for solving important problems as well as to use the knowledge for reapplication. Indeed, the ontology as a general scheme for presentation and usage of knowledge can not only clearly be defined for agents working with it (as with the shared resource), but also shared between agents, as well as replicated. We should also note that the corresponding knowledges are generated according to the approach described above (see Fig. 2) and corresponding information should be stored in the special data and knowledge bases.

Thus, the use of ontology involves direct work with ontological user model. With expansion and evolution of ideas on the subject area during work, ontology should be updated as well. Accordingly, an important requirement for system maintenance of ontologies is to provide their support editing operations and expansion of the existing ontologies. In addition, the applicative use of ontologies involves interaction with ontological system of software agents, providing users requests processing and implementing the interaction of components of distributed applications. In other words, the above mathematical models under-

[1] http://www.magenta-technology.ru/.

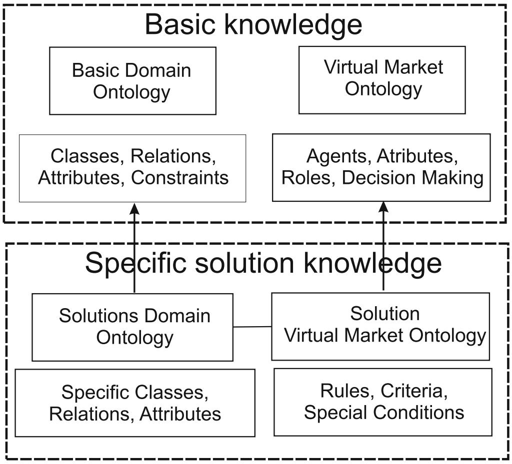

Fig. 3. The ontologies types.

lying Lego-objects technologies give users the ability to work with the ontological model, thus providing support for the necessary operations for creating, editing and ontology extension the subject area.

To support the operation and modernization of distributed intelligent systems, performing the operations described above (i. e., thereby functioning ontologies) must meet the following requirements:

– reliable semantic basis in determining the content of information;
– general logical theory, which consists of a "dictionary" and set of statements, implemented using some logical language;
– reference tool to provide the necessary communication both between users and computer agents, as well as between agents.

To implement the necessary operations we should use a special tool for editing ontologies (in particular, on the site of W3C several dozen tools for editing ontologies are provided).

3.3 The Problems of Data Processing

The approach described above also requires efficient data processing techniques. Specifics of the problems under consideration, and the proposed approach demand effective methods for solving the corresponding problems. Required data collection process becomes a very large and complex problem, and it gets difficult to process using relatively traditional database management tools or traditional data-processing applications.

In particular, similar problems include such special tools as data capture, monitoring, storage, retrieval, exchange, transfer, analysis, and visualization. The above-discussed concept of multi-agent systems is connected with the necessity of processing additional information obtained from the analysis of a large intermediate set of related data. Researchers are constantly faced with limitations in the computational procedures that are primarily associated with large volumes of data.

In the process of developing and implementing particle beams management systems, researchers are faced with the need to deal with the enormous number of data coming from the accelerator as a control system, and also from the beam itself. Thus, we obtain two sets of data that must be processed and implemented using the corresponding control processes. The first data set contains the data of numerical simulation, the second – the corresponding experimental data.

Effectiveness of these manipulations is largely determined by both modeling techniques used (in this case, the use of multi-agent systems within the concept of Lego-objects) and software methods implemented in the necessary procedures to process arrays of data obtained both in the working functioning and in numerical modeling.

The second set of data is associated with the measurement data, such as the monitoring control system and state of the beam. The harmonization of these data sets, their consolidation, storage and processing can be implemented effectively within the Big Data ideology. Moreover, since the physics accelerators become relatively common international mega projects, then the required data volume repeatedly increases.

In this case we have in mind the final data set (the end result of simulation) as well as an intermediate (current) one, which volume is much higher. It should be noted that the volume of such data is increased significantly in the study of particle beams dynamics with the influence of the self-field of the beam (for intense beams). Processing such data may be conducted within the concept of Virtual Accelerator.

4 Conclusion

In this article, we described a technique matching the physical essence of the modeled area of knowledge (in our case the beam physics in accelerators) with modern technologies, high performance computing through the use of multi-agent technologies. In the cited works, the solution of similar problems with usage of the matrix formalism for Lie algebraic methods has led to the possibility of introducing the concept of global optimization methods [12] in the structure of modern computing. Indeed, multiparametric character of the modern control systems for accelerator complexes leads to the need for use of multi-agent technologies as a tool for finding optimal solutions in multidimensional space of control parameters. The main advantages of multi-agent systems consist not only in processing of distributed information, but also in using the principles of intelligent processing of the corresponding information. Efficiency of implementation of multi-agent-based approach is largely determined by the choice of the mathematical tools. The matrix formalism for Lie methods allows to optimally adapt methods used for describing of the dynamics of particles in accelerators to the ideology of multi-agent systems. It should also be noted that the proposed mathematical and informational models necessitate the use of advanced technology in distributed data processing both in the processing and storage of data.

Acknowledgements. The work is supported by Saint Petersburg State University (project 0.37.155.2014).

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