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as a manuscript

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Study of Virtual Time Models in Parallel Discrete Event Simulation Algorithms

PhD disseration summary

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The relevance of research

The leading countries need in high-performance computing is continuously growing. The high-performance systems are used in machine learning, material sciences, cosmology, computational physics and chemistry, bioinformatics, etc. The development and implementation of modern technologies influence the ability of countries and companies to solve important problems in science, engineering, economic, etc.

The performance of modern supercomputers reaches hundreds of Teraflops (1Tp = 1 million operations per second). For the effective use of such powerful systems, one needs to develop new parallel algorithms, compilators, libraries, and other instruments.

The method studied in the dissertation is known as the parallel discrete event simulation (PDES) method. PDES is a universal instrumental tool, which allows running one simulation program on the number of computational nodes (CPU/cores/threads). The method is widely used in supercomputer modeling to solve fundamental problems in science as well as applied tasks in economics, medicine, sociology, etc. Moreover, the PDES method is constantly enhancing by developing new algorithms and useful frameworks for visualization and analysis of PDES models.

Problem statement

One of the simulation problems is that the behavior of a particular parallel model highly depends on the hardware architecture. Therefore, before running a large-scale simulation, it is better to study the model and choose optimal parameters first. The scalability and performance of the particular model must be studied before the large-scale simulation. Moreover, such a study itself my be also resource-intensive.

In the dissertation we study the properties of PDES models, regardless of the subject area and the hardware architecture. In the research, we build and study the models of local virtual time profile evolution in different parallel discrete event simulation algorithms. The models may be used for the prediction of performance and scalability properties of real simulation models. The prediction is based on the behavior of the local virtual time profile in the algorithms.

A brief description of the PDES method. In the parallel discrete event simulation, one simulation task is split into subtasks, which are run by their *logical processes* (sequential subprograms). The state of the simulated system changes at some instants of time. Such changes are called *discrete events*. Each logical process is characterized by its local virtual time (LVT) and has a local queue of events. The logical process works in a cycle, taking events from the queue and processing them in time-stamped order. In modern PDES systems number of processed events reaches hundreds of millions per second. Logical processes can also generate events for other processes. The parallel processes communicate by sending time-stamped messages containing information about events. For ensuring the correctness of parallel simulation all events in the system must be processed in time-stamped order. This is done by special synchronization mechanisms, which are classified into three groups: conservative, optimistic and Freeze-and-shift (FaS) algorithms.

The object of the research is a set of all local virtual times (Figure 1), which is called the local virtual times (LVT) profile. The LVT profile evolves during the simulation and at any time instant can be described by two observables: the average virtual time, and the average width (the standard deviation). Depending on the synchronization algorithm and communication topology, the behavior of the LVT profile differs. We build models of the evolution of the LVT profile for conservative and optimistic synchronization algorithms on different topologies. We study the dependence of the average speed of the profile and the average width of the profile on the number of logical processes and the fraction of distant communications between them. These observables allow us to predict the effectiveness and scalability of the models. The average speed of the profile reflects the utilization of events, and the average width of the profile reflects the desynchronization between parallel processes.

The aim of the dissertation research is studying of the models of evolution of LVT profile in different parallel discrete event simulation synchronization algorithms and on different communication topologies.

For the achievement of a goal the following research tasks are formulated:

1. Developing the model of the evolution of the LVT profile in a conservative PDES algorithm on 1+1 dimension (space+time) on small-world topology.

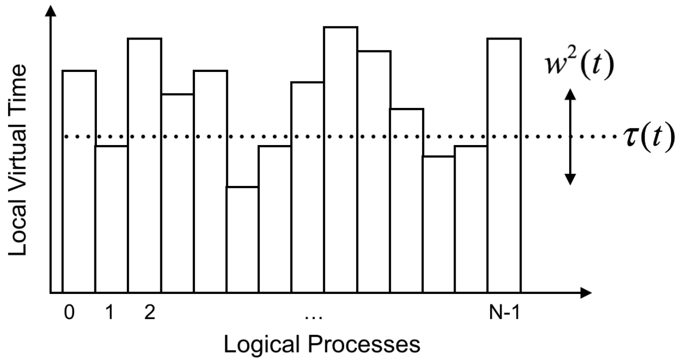

Figure 1: The LVT profile at some fixed instant of simulation time. Each logical process has its value of LVT. $\tau(t)$ is an average LVT, and $\tau(t)$ is a standard deviation from the average LVT.

2. Developing the model of the evolution of the LVT profile in an optimistic PDES algorithm on 1+1 dimension (space+time) on regular and small-world topologies.

3. Studying the behavior of the average speed and the average width of LVT in the models depending on the topology and the number of logical processes.

4. Studying the models on their belonging to the universality classes in physics.

5. Checking models for the adequacy. Establishment of the correspondence between the simulation results and the experimental data obtained using the ROSS simulator (a framework for parallel discrete event simulations).

Degree of problem development

The approach to the study of effectiveness and scalability of the PDES algorithms via the analysis of the LVT profile evolution was proposed by Korniss' scientific group [Korniss G. et al., Phys. Rev. Lett. 84(6), 1351, 2000]. The authors proposed a model of the evolution of the LVT profile in the conservative algorithm on one-dimension topology with periodic boundary conditions. In this topology, the local processes interact only with the nearest neighbors. Each logical process is mapped on one processing element (CPU/core/thread). The authors drew an analogy between the local virtual time profile and the nonequilibrium surface growth. The random local increase of virtual time in the model of the conservative algorithm corresponds to the deposition of a random amount of material in the local minimum of the growing surface (for example, as in molecular-beam epitaxy).

The authors showed that on a regular one-dimensional topology, the growth of the LVT profile in the conservative algorithm can be described by the Kardar-Parisi-Zhang equation (KPZ). The efficiency of the algorithm, in this case, corresponds to the density of the local minima of the LVT profile. Simulation of the evolution of the LVT profile in a conservative algorithm and a coarse-grained approximation showed that the algorithm is asymptotically scalable, i.e. as the number of logical processes increases, the velocity of the profile growth remains nonzero, but the width of the LVT profile diverges. A nonzero growth rate of the LVT profile means that the conservative algorithm is free from deadlocks, while the growing profile width indicates the increasing desynchronization between parallel processes. The analogy between the local time profile in PDES and surface growth made it possible to attribute the model of the growth of the LVT profile in the conservative algorithm with local interactions to the KPZ universality class and predict properties of the algorithm in the limit of an infinite number of logical processes.

Another important consequence of the established analogy of the local time evolution model in the conservative PDES algorithm and surface growth in physics is that all PDES synchronization algorithms were classified into three classes – conservative, optimistic, and Freeze-and-Shift (FaS) algorithms, corresponding to the periodic, open, and fixed boundary conditions of the KPZ equation [Shchur LN, Novotny MA Phys. Rev. E., 70 (2), 026703, 2004].

The topology of the logical processes plays an important role in the analysis of PDES models performance. The first model of LVT evolution in the conservative PDES algorithm took into account only local interactions between the parallel processes. In real models, besides the local interactions, long-distance communications between the logical processes may also occur. In later works of the Korniss' group, for example, in [Guclu H. et l., Phys. Rev. E. 73 (6), 066115, 2006], the influence of a small number of random long-range interactions on the synchronization aspects in the conservative PDES algorithm has been studied. The simulation of the LVT profile growth was carried out on a topology, which has similar properties with small-world topology. The addition of a small number of random long-distance interactions between LPs significantly reduces the width of the LVT profile, while the average speed of the profile remains positive. The conservative algorithm on such a topology becomes fully scalable: in the limit of an infinite number of logical processes, the average width of the LVT profile remains constant (and does not grow, as on a regular topology), while the average speed decreases slightly.

The effectiveness of parallel discrete-event simulation is also studied on particular case-studies of PDES models on special frameworks such as ROSS, PDEV, μsik, etc. The performance analysis of the specific models is measured in terms of the number of processed events per time unit. The disadvantage of such approach is that such studies are hardware and model-dependent and their results are not universal.

The scientific novelty of the study

The scientific novelty of the study is in the application of such a well-known method of studying the PDES method, as modeling the evolution of the LVT profile, to new synchronization algorithms with a new interaction topology of logical processes. In addition, for the first time, in the dissertation research, the data obtained during the simulation of LVT profile is compared with the results of running a real model on the ROSS simulator.

The scientific novelty of the study is described in more detail in the following paragraphs.

Firstly, during the dissertation research, we built and studied the model of the evolution of LVT profile in the conservative PDES algorithm on the small-world topology. We also compare our results with the results of Korniss' works, where the analysis of the influence of a small amount of random long-range interactions between LP has been done. In the Korniss' model each LP is conntected with exactly three nodes, two of which are the nearest neighbors, and one is randomly selected from the remaining distant LPs. The long-distance connections are "turned on" with a probability of p.

Such a model has some properties of small-world topology, but it is not a small-world topology by definition [Watts, Strogatz, Nature, 393 (6684), 440, 1998]. In our work, we build a small-world topology using standard algorithms.

First, the LPs are connected into a regular topology, and then long-range interactions are added (or rewired from the short-range connections) randomly with probability p. This method of constructing a network with the properties of a small-world is classical and such topology better reflects the properties of real simulated systems. Thus, the scientific novelty of this part of the work is in the choice of a more natural interaction topology between LPs.

Secondly, in the dissertation, for the first time, a model for the evolution of the LVT profile for the optimistic PDES algorithm is proposed. The model is studied on the regular and small-world topologies. As a result of the study, it was shown that the model of the optimistic PDES algorithm can be attributed to the Directed Percolation (DP) universality class in physics.

Thirdly, no one has previously studied the behavior of local virtual times in real PDES models. Typically, the performance of parallel discrete event simulation is measured in the number of events processed per time unit. We asked the developers of the ROSS simulation framework to add an option to output local virtual times of the processes in statistics, which made it possible to verify the model studied in the dissertation for agreement with real simulations.

Thesis statements for defending

1. The model of evolution of LVT profile in conservative PDES algorithm has been built and studied on different variations of small-world topologies.

2. The dependence of the average speed and the average width of the LVT profile on the fraction of long-range interactions p between logical processes has been established.

3. The model of evolution of LVT profile in optimistic PDES algorithm has been proposed and studied on regular topology and different variations of small-world topologies.

4. It has been shown that the model of the LVT evolution in optimistic PDES algorithm belongs to the directed percolation universality class.

5. The correspondence between the simulation results and the experimental data obtained using the ROSS simulator has been established.

Personal contribution of the author. The ideas in the dissertation were proposed by the author together with the academic supervisor. The author personally has developed the program code, made numerical experiments and processed the results. The author has made the main contribution to the writing of scientific articles on the topic of the research.

Degree of reliability of the results. The research made by the applicant for the scientific degree is confirmed by a number of numerical experiments and discussions in scientific groups. The results of the dissertation research have been presented at numerous conferences and published in leading scientific journals.

Theoretical significance of the work. In the dissertation research, the mathematical models of the evolution of the local virtual times in PDES algorithms are proposed. It is shown that these models can be used to predict the scalability and efficiency properties of parallel discrete event simulation models. The properties of these models on the regular topology and the topology of the small world are studied in detail. The author has drawn an analogy of the models with models of surface growth in physics and attributed them to the universality classes in physics.

Practical significance of the work. The models proposed in the dissertation can be used to predict the properties of scalability and efficiency of real parallel discrete event simulation models. The fact that these models belong to the universality classes allows the use of well-developed instruments of statistical physics for further study and prediction of the behavior of PDES models.

General findings of the study

The main findings of the dissertation research are the following:

1. For the first time, a model of the growth of virtual times in a conservative algorithm on the small world topology has been studied. The functional dependence of the average speed and the average width of the LVT profile on the concentration of long-range interactions p was revealed. It was shown that the speed of the profile is mainly affected by the number of interactions between

logical processes, while the clustering coefficient has no qualitative impact on the behavior of the model. The dependence of the model behavior on the local connectivity of the network was also studied in detail. Also, the results were compared with the results of similar works of other scientific groups.

2. A model for the evolution of local virtual times profile for the optimistic PDES algorithm has been developed and studied. The model has been examined on the regular and small-world topologies. We studied the phase transition between the active and absorbing phases of the LVT profile growth. In the active phase, the local virtual time profile grows with a nonzero rate. As the the parameter q ("growth rate") decreases, the average speed of the profile v is also decreasing to zero as $v = v_0(q - q_c)^\nu$. The critical point q_c and the critical exponent ν were calculated. The study showed that the model for the optimistic PDES algorithm can be attributed to the directed percolation universality class.

3. The adequacy of the LVT profile growth model in the optimistic algorithm is verified. In the dissertation, for the first time, the analysis of the behavior of LVT in real PDES models on ROSS simulator is studied. A comparison of the proposed model for the optimistic algorithm with the PCS (Personal Communication Service) communication network model, running on the ROSS framework, showed that the growth rate of the LVT profile in the model for the optimistic algorithm does reflect the simulation performance. The average speed of the local virtual time profile in both cases decreases with the parameters p and q and has a phase transition at the point q_c. The critical point q_c for the OSW and PCS models coincides, as well as the critical exponent ν. The qualitative behavior of the average width of the LVT profile in both models also coincides.

The results of the dissertation research have high theoretical and practical significance. The models proposed and studied in the dissertation can be used to predict the properties of scalability and efficiency of parallel discrete event simulation models. The analogy of models with models of surface growth in physics allows the use of a well-developed apparatus of statistical physics for further study and prediction of their behavior.

Aapprobation of the results

The work underwent approbation at the following conferences:

1. The 5th International Conference on Matrix Methods in Mathematics and applications, «On the properties of parallel discrete event simulation algorithms», Moscow, August 19-23, 2019;

2. International Conference on Computer Simulation in Physics and beyond, «The analysis of optimistic parallel discrete event simulation algorithm on small-world networks», Moscow, September 24-27, 2018;

3. The 8th International Conference «Distributed Computing and Grid-technologies in Science and Education», «Synuchronization aspects on the optimistic parallel discrete event simulation algorithms», Dubna, Russia, September 10-14, 2018;

4. International Conference on Computer Simulation in Physics and beyond, «The analysis of conservative and optimistic parallel discrete event simulation algorithms on small-world networks», Moscow, October 9-12, 2017;

5. The 14th International Conference on Parallel Computing Technologies, «Properties of the conservative parallel discrete event simulation algorithm», Nizhniy Novgorod, Russia, September 4-8, 2017;

6. The Sixth China-Russia Conference on Numerical Algebra with Applications, «Analysis of Local Virtual Time Profile in Parallel Discrete Event Simulation», Moscow, August 28–30, 2017;

7. XXIX IUPAP Conference in Computational Physics, «Synchronisation of Conservative Parallel Discrete Event Simulations in Small World Network», Paris, July 9-13, 2017;

8. Landau Days, «Synchronisation in parallel event simulation algorithm on the small-world network», Chernogolovka, Russia, June 26-29, 2017;

9. International Conference «Supercomputer Simulations in Science and Engineering», «Simulation of virtual time profile in conservative parallel discrete event simulation algorithms for small-world network>, Moscow, September 6-10, 2016;

10. International Conference on Computer Simulation in Physics and beyond, «Virtual Time Profile Modeling in Parallel Discrete Event Simulation», Moscow, September 6-10, 2015.

The list of the published articles where the main scientific results of the thesis are reflected

The main results of the dissertation are reflected in the following works.

The list of articles published in the journals included in international citation system WoS or Scopus:

1. Ziganurova L., Novotny M. A., Shchur L. N. Model for the evolution of the time profile in optimistic parallel discrete event simulations //Journal of Physics: Conference Series, 681(1), 012047 (2016) (WoS, Scopus Q3).

2. Shchur L., Ziganurova L. Simulation of virtual time profile in conservative parallel discrete event simulation algorithm for small-world network // Lobachevskii Journal of Mathematics, 38(5), 967-970 (2017) (WoS, Scopus Q3)

3. Ziganurova L., Shchur L. Properties of the Conservative Parallel Discrete Event Simulation Algorithm. In: Malyshkin V. (eds) Parallel Computing Technologies. PaCT 2017. Lecture Notes in Computer Science, vol 10421. Springer, Cham (2017) (WoS Q4, Scopus Q2)

4. Ziganurova, L., Shchur, L. N. Synchronization of conservative parallel discrete event simulations on a small-world network // Physical Review E, 98(2), 022218 (2018) (WoS Q1, Scopus Q1)

5. Ziganurova L., Shchur L. Properties of The Parallel Discrete Event Simulation Algorithms on Small-World Communication Networks in Proceedings of the VIII International Conference “Distributed Computing and Grid-technologies in Science and Education”, 2267, 70-75 (2018) (Scopus)

6. Shchur L.N., Ziganurova L.F. Synchronization of Processes in Parallel Discrete Event Simulation // Journal of Experimental and Theoretical Physics, Vol. 129, No. 4, pp. 722–732 (2019) (WoS, Scopus Q2)

7. Ziganurova L., Shchur L. Synchronization Aspects of The Optimistic Parallel Discrete Event Simulation Algorithms, in Data Analytics and Management in Data Intensive Domains eds. A. Elizarov, B.Novikov, S. Stupnikov, p.182 (paper 18) (Scopus)

The list of articles published in the journals included in Russian Science Citation Index

1. (in Russian:) L. F. Ziganurova, L. N. Shchur Study of the conservative algorithm of parallel discrete event simulation on Small-world networks // // Computational technologies in sciences: supercomputer modeling methods, part 4., pp. 28-34 (2017)

2. (in Russian:) E.V. Khomutov, L. F. Ziganurova The analysis of the virtual local time in optimistic parallel discrete event simulation algorithm // New information technologies in automated systems: materials of the twenty-first scientific and practical seminar. M .: Institute of Applied Mathematics. M.V. Keldysh RAS, 2018.S. 294-299. (2018)

Certificate of state registration of software

1. Certificate of state registration of software №2016663469 “Simulation of conservative synchronization algorithm in parallel discrete event simulation on Small-world topology”

2. Certificate of state registration of software №2017662914 “Simulation of Small-world topology”