REVIEW

On the procedure for defense of PhD thesis entitled:

„Porous Medium Flow Simulations Using Massively Parallel MLMC Algorithm"

For acquisition of the educational and scientific degree "Doctor"

by

<u>PhD student</u>: **Nikolay Georgiev Shegunov,**

<u>Area of higher education</u>:   **4. Natural Sciences, Mathematics and Informatics**

<u>Professional field</u>**:**   **4.6. Informatics and Computer Sciences**

<u>PhD program</u>: **„Information Systems",**

<u>Department</u>: **„Computer Informatics", Faculty of Mathematics and Informatics (FMI), Sofia University „St. Kliment Ohridski"(SU)**

<u>Reviewer</u>: **Professor Dr. Todor Gurov from the Institute of Information and Communication Technologies at the Bulgarian Academy of Sciences (IICT-BAS), Member of the scientific jury in accordance with Order № PD 38-258 /07.06.2021 by the Rector of Sofia University**

1. General characteristics of the PhD thesis and of the presented materials

The presented materials have been prepared in accordance with the Development of Academic Staff in the Republic of Bulgaria Act (DASRBA), the Regulation for the Application of (DASRBA), as well as with Rules for the Conditions and Procedure for Acquisition of Scientific Degrees and Occupation of Academic Positions (RCPASDOAP) in Sofia University. They include: 1) PhD Thesis in English; 2) Abstract in Bulgarian and English; 3) Copy of the master's degree diploma; 4) Copies of the scientific publications on the topic of the PhD thesis 5) Information on fulfillment of the minimum requirements according to the Regulation for the Application of DASRBA; 6) List of scientific publications on the topic of the dissertation; 7) Declaration of Nikolay Shegunov's co-authors for his contribution to one of their publications; 8) Curriculum vitae in Bulgarian and English; 9) Authentication Protocol and Opinion on the

procedure for prevention of plagiarism, signed by his supervisor; 10) Report extracted through the software product StrikePlagiarism.com on the lack of plagiarism; 11) Declaration from Nikolay Shegunov for originality and lack of plagiarism.

The dissertation consists of: 1) 6 /six/ Chapters; 2) 3 /three/ Appendices, including a list of abbreviations, description of the computing resources and a list of 43 figures and 20 tables; 3) Bibliography with 62 titles, and 4) Declaration of Originality. The total volume of this PhD thesis is 129 pages.

The dissertation is devoted to the development, research and testing of massive MLMC algorithms for simulation of flows in the porous medium. Mathematical models describing flows in the porous medium are presented by 1) Laplace equation and 2) convection-reaction-diffusion equation.

2. Data and personal impressions for the PhD candidate

Nikolay Shegunov was born on May 15, 1990 in the city of Sofia, Bulgaria. In 2013 he has graduated from FMI-SU with a bachelor's degree in Informatics. In 2015 Shegunov has got MSc degree in the program "Computational Mathematics and Mathematical modeling" again from FMI-SU. As a student he has visited the University of Karlsruhe, Germany, under the European Erasmus Student Exchange Program. He is currently working at FMI-SU, participating in conducting basic programming courses. By Order № PD 20-877/23.06.2020 of the Rector of Sofia University he was enrolled as a doctoral student in independent training at the Faculty of Mathematics and Informatics with supervisor Assoc. Prof. Dr. Petar Armyanov from the Department of Computer Informatics. He is currently working at FMI-SU, participating in basic programming courses.

3. Analysis of the scientific and scientific-applied achievements of the candidate, contained in the presented dissertation and the publications to it, included in the procedure

In the first chapter, the doctoral student has motivated the need of a Multilevel Monte Carlo (MLMC) algorithm for solving problems describing the simulation of flows in porous medium. He has stressed that such type of algorithms is successfully applied to NP-hard problems, which describes porous mediaflow modeling. Various methods used in stochastics to study problems

with uncertainties are also considered. Modern HPC systems with distributed, shared and hybrid memory are also described in this chapter, as well as some software products and libraries needed for his work. At the end of the chapter the main aim of the dissertation has defined, namely, to develop and study a massively parallel version of a MLMC algorithm for solving two partial differential equations defined in probability space and describing the simulation of flows in porous medium.

In the second chapter the methodology has been described that is used to solve the considered differential equations. This methodology includes the finite volume method applied for discretization of given PDEs and a MLMC algorithm for solving the corresponding discrete problem. Various generating algorithms have been considered for sampling values of random variables with given distributions. Finally, two important properties, that characterizes a porous medium are introduced, namely, porosity and permeability.

In the third chapter a Laplace equation is considered describing a steady state single phase flow in a random porous media. The finite volume method is applied for its discretization and MLMC algorithm is constructed for estimating the solutions of the discretized problem.

In the fourth chapter of the dissertation a problem describing a reactive transport inside a random porous medium is considered. The mathematical model is presented by a convection-reaction-diffusion equation. Again as in the previous chapter the finite volume method is used for discretization and MLMC algorithm is constructed to solve the discretization problem. The numerical results presented in these two chapters demonstrate the advantages of the MLMC algorithm compared to the classical MC one.

A fifth chapter is devoted to the development and research of the parallel MLMC algorithm for solving the above two equations. The main results of the dissertation are presented here. A block diagram of the parallel algorithm is constructed and several parallel strategies for its implementation are described in detail.

The numerical results obtained on various HPC computing resources (see Appendix B) demonstrate the need to apply an appropriate parallel strategy depending on the given problems and the computer architecture used. The obtained results are summarized in **the chapter 6** and some guidelines have been pointed for future research. The list of publications on the dissertation is also presented.

Overall, I appreciate the PhD student's contributions as scientific and applied ones.

4. Approbation of the results

The results of the dissertation are published in 5 papers, all are in English. A brief analysis of these publications shows the following:

- 1 publication is in a journal (№ 5, from the list of papers in the abstract).
- 3 publications are in conference proceedings published by Springer (№№ 1, 3, 4).
- 1 publication is in a conference book available in a repository with Open Access (№2).
- All publications are indexed in Scopus, 4 of them are with SJR index and Q2 quartiles (№№ 1, 3, 4, 5), and one (№ 2) is without SJR index.
- All publications are co-authored.

Signed declaration was submitted by the co-authors for the paper №2 that the main contribution of the doctoral candidate Nikolay Shegunov is estimated at 80%. I accept that all authors in the other 4 papers have an equal contribution.

The scientific indicator compared to the minimum requirements (30 points) for the educational and scientific degree "Doctor", according to the Regulation for the Application of DASRBA (p. 27) is as follows: All publications fall into the G7 group and they accumulate 77.83 points total. Each publication is evaluated with 40 points divided by the number of the authors. The paper №2 is evaluated with 32 point, because the candidate's contribution is 80%.

Based on the presented materials, the reviewer accepts there is no legally proven plagiarism in the PhD thesis and in the scientific papers on this procedure.

5. Qualities of the abstract

The abstract, presented in Bulgarian and English has a volume of 40 pages. It reflects the content of the dissertation and complies with DASRBA, the Regulation for the Application of DASRBA, as well as with RCPASDOAP in Sofia University.

6. Critical comments and recommendations

The dissertation is relatively well balanced, but it would be good if the author's contributions are better formulated. For example, the first scientific contribution, according to the doctoral student, is related to a review and analysis of the existing solutions to the problems. This contribution is related to the educational part of the doctoral student rather than the scientific one.

In my opinion, the second chapter is related to the methodology used and it should not have been entitled "Mathematical Models". There are scientific terms in the Bulgarian version of the abstract that have not been translated from English correctly.

I would noted that due to differences in the hardware characteristics of the NVIDIA Tesla K80 GPUs card and Intel Xeon E5-2695 v2 processor, it is normal to get the described acceleration in favor of the GPU card. The important performance specifications of the NVIDIA Tesla K80 GPA accelerator include: aggregate memory bandwidth of 480GB/sec and 2.91 Tflop/s double precision with GPU Boost, while the important performance specifications of Intel Xeon E5-2695 v2 processor are: 59.7 GB/s max memory bandwidth and about 150 Gflop/s pick performance.

My recommendation here is as a future work to be investigated the energy efficiency when GPU cores and CPU cores are used. I also recommend the doctoral student to be more precise in his speech in the next publications and descriptions of scientific results.

7. Conclusion

The results obtaining on the topic of the PhD thesis show that the doctoral candidate Nikolay Shegunov has theoretical knowledge and practical skills in the field of informatics and computer science. The presented dissertation meets the requirements of DASRBA, the Regulation for the Application of DASRBA, as well as the Rules for the Conditions and Procedure for Acquisition of Scientific Degrees and Occupation of Academic Positions in Sofia University. In particular, the published papers under this procedure cover the minimum national requirements, even exceeding them a few times.

Based on the above, I recommend the honorable Scientific Jury to award **Nikolay Georgiev Shegunov** with the Educational and Scientific Degree "Doctor" in the area of the higher education: **4. Natural sciences, mathematics and informatics**, a professional field: **4.6. Informatics and computer science**.

15.08. 2021.   **Reviewer: ....**

                                        (Professor Dr. Todor Gurov)