OPINION

from Prof. Dr. Aneta Karaivanova Institute of Information and Communication Technologies - BAS Member of the Scientific Jury appointed by the Rector of SU "St. Kliment Ohridski" via Order № РД-38-258/07.06.2021

SUBJECT: Dissertation of Nikolay Georgiev Shegunov entitled "*Porous Medium Flow Simulations using Massively Parallel MLMC algorithm*" presented for the acquisition of educational and scientific degree "Doctor" in the professional field 4.6 Informatics and Computer Science, Doctoral Program "Information Systems" with supervisor Assoc. Prof. Petar Armyanov (Sofia University) and scientific consultant Prof. Oleg Iliev (University of Kaiserslautern, Germany).

1. General description

The materials presented for an opinion include all documents required by the Law on the Development of the Academic Staff in the Republic of Bulgaria, the Rules of its implementation, the Rules for the conditions for the acquisition of academic degrees and for the occupation of academic positions in the Sofia University, and the requirements of Faculty of Mathematics and Informatics. The dissertation is presented in 6 chapters on 129 pages, written in English, and contains 44 figures, 20 tables and bibliography with 62 sources. The extended abstract is written in Bulgarian, on 37 pages. The publications are published in the period 2017-2020, and 4 of them are with SJR rank.

Nikolay Shegunov has graduated the Sofia University (Faculty of Mathematics and Informatics) with Bachelor Degree in Informatics in 2013 and with MSc Degree in "Computational Mathematics and Mathematical Modelling" in 2015. As a student he participated in Erasmus program studying in Karlsruhe University. He was enrolled for individual doctoral study on 25.06.2020 and deducted with the right of defense on 21.05.2021. The dissertation was discussed and scheduled for defense on a seminar of the Department of Computer Informatics at FMI.

2. Relevance, significance and goals of the dissertation

The dissertation is devoted to application of Multilevel Monte Carlo (MLMC) algorithm for study the porous media flows and development of an efficient parallel realization of the algorithm. The MLMC algorithm is first suggested by Stephan Heinrich in several publications in the period 1997-2000 for computing $E[f(x; \lambda)]$, where x is a random variable and λ is a parameter, and after that has been successfully applied in various domains.

To achieve the dissertation goals the following tasks are considered:

• Explore the existing approaches to the problem.

- Choose effective algorithm for generation of random porous medium permeability fields.
- Provide an efficient coarsening strategies for the MLMC setting.
- Provide an adequate heuristic algorithm for efficient work scheduling.
- Choose appropriate software for effective implementation in HPC setting.

3. Main results in the dissertation and their approbation

In chapter 2 the necessary mathematical foundations needed for the simulations are presented. The general form of MLMC is given, including analysis of its computational cost. In chapter 3 a simple stochastic Laplace equation model is presented. This stochastic partial differential equation is well established as a model equation in the field of uncertainty quantification in porous medium flows and shows well the computational and modeling challenges of applying Multilevel Monte Carlo algorithms. Chapter 4 considers a practical example of transport of mass within a porous media. The formulated equation has much higher computational complexity than the Laplace equation. It is widely used and has many application areas as building block in more complex models. The final chapter 5 considers the programming aspect of the problem. In it the algorithm procedure for computation is formulated and different scheduling strategies are considered capable of utilizing a large number of processor cores. The chapter ends with experiments and analysis of the proposed algorithms. Each chapter finishes with a conclusion section, consisting of a summary with the key points in the chapter.

Four of the publications containing main results of the dissertation have been presented at large scientific conferences. Mr. Shegunov has also given 2 seminar talks.

4. Scientific contributions

The scientific and applied contributions of the dissertation are contained mainly in Chapters 3, 4 and 5. I accept the summary made by the doctoral student in Chapter 6:

- Scientific contributions:
 - A review and analysis of the existing solutions to the considered problems are made. The advantages and disadvantages of the existing solutions for generating stochastic fields and corresponding sampling algorithms are evaluated (Chapter 2);
 - Different approaches for approximation of the stochastic field for the Laplace problem are analyzed and compared (Chapter 3);
 - An effective method for renormalization of the stochastic field for the purposes of the Multilevel Monte Carlo has been developed (Chapter 3);
 - An adaptive algorithm for resource allocation between the different levels of the Multilevel Monte Carlo algorithm has been developed (Chapter 5);
 - The Multilevel Monte Carlo method is applied successfully for the first time to solve the convection-reaction-diffusion equation (Chapter 4).
- Scientific and applied contributions

- An approach for determining the levels for the Multilevel Monte Carlo for the two considered problems is defined (Chapter 3 and Chapter 4);
- Analysis and comparison of the two considered approaches for coarse grain, for the Multilevel Monte Carlo versus the classical Monte Carlo for the convection-reaction-diffusion problem are performed (Chapter 4);
- Analysis and comparison between the rate of convergence and the time for calculation of the Multilevel Monte Carlo method with simplified renormalization and the classical Monte Carlo are made (Chapter 3);
- An overview, analysis and comparison of six parallelization strategies are made (Chapter 5).
- Applied contributions
 - A strategy for generating random fields on graphic accelerators has been developed and implemented (Chapter 5);
 - Four advanced parallel algorithms were proposed, implemented and compared (Chapter 5);
 - The applicability of the considered approaches for large scale simulations of realistic problems was confirmed with tests on a large number of cores (Chapter 5).

5. Opinion on the extended abstract

The presented abstract of the dissertation correctly reflects the content and results presented in the dissertation.

6. Critical remarks

I have no critical remarks. There are some minor technical mistakes, and insignificant translation errors.

7. Personal impressions

I have no personal impressions from Mr. Shegunov.

CONCLUSION

The presented dissertation meets the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria, the Rules of its implementation and the Rules for the conditions for the acquisition of academic degrees and for the occupation of academic positions in the Sofia University.

The obtained results in the dissertation and the fulfillment of the national minimum requirements give me enough reason to give a positive assessment of the dissertation work and *I suggest to the honorable scientific jury to award to Nikolay Shegunov the educational and scientific degree 'Doctor'' in Doctoral program ''Information Systems'' professional field 4.6 Informatics and Computer Science.*

15.08.2021

Signature:

/Prof. A. Karaivanova/