Резюмета на научните публикации за участие в конкурса - на английски на

на д-р Тодор Василев Гюров, доцент в ИИКТ-БАН

представени за участие в конкурса за академичната длъжност "професор" по професионално направление 4.5. Математика, специалност "Математическо моделиране и приложение на математиката (Монте Карло и квази-Монте Карло алгоритми и приложения)", обявен в ДВ бр. 41 от 21 май 2019 г,

Публикации включени в групов показател В, точка 4. (6 броя)

Atanassov, E., Gurov, T., Karaivanova, A.. Energy aware performance study for a class of computationally intensive Monte Carlo algorithms. Computers and Mathematics with Applications, 70, 11, Elsevier, 2015, DOI:10.1016/j.camwa.2015.07.014, 2719-2725. ISI IF:1.697, <u>Линк</u>.

The latest developments in the domain of HPC have lead to the deployment of complex extreme-scale systems, based on diverse computing devices (CPUs, GPUs, accelerators) thus posing the question of scalability in the light not only of parallel efficiency, but also in terms of energy efficiency. In this paper we propose new metrics for energy aware performance estimation based on our experience and the analysis of the existing metrics. We study the performance of computationally intensive Monte Carlo applications deployed on heterogeneous HPC systems with focus on energy efficiency and equipment costs. We compare the energy aware performance results of CPU and GPU variants of the tested algorithms with respect to the introduced measures and metrics. The results of our study demonstrate the importance of taking into account not only scalability of the HPC applications but also energy efficiency and equipment cost. They also show how to optimize the selection of CPU computing or computing with GPGPUs. The results can be used by application developers/users and also by resource providers.

 Atanassov, E., Gurov, T., Karaivanova, A., Nedjalkov, M., Vasilevska, D., Raleva, K.. Electron-phonon interaction in nanowires: A Monte Carlo study of the effect of the field. Mathematics and Computers in Simulation, 81, 3, 2010, DOI:10.1016/j.matcom.2009.09.006, 515-521. ISI IF:1.476, <u>Линк</u>

The femtosecond dynamics of highly non-equilibrium, confined carriers is analyzed within a Monte Carlo approach. The physical process considered corresponds to a locally excited or injected into a semiconductor nanowire distribution of heated carriers, which evolve under the action of an applied electric field. The carriers are cooled down by dissipation processes caused by phonons. The process is described by a quantum-kinetic equation which generalizes the classical Boltzmann equation with respect to two classical assumptions, namely for temporal and spatial locality of the carrier-phonon interaction. We investigate the effect of the field on the electron-phonon interaction - the intra-collisional field effect (ICFE). A Monte Carlo method for simulation of the considered process has been utilized. Simulation results for carrier evolution in a GaAs nanowire are obtained and analyzed for phenomena related to the ICFE.

 Dimov, I. T., Gurov, T. V., Penzov, A. A. A Monte Carlo Approach for the Cook-Torrance model. Lecture Notes in Computer Science, 3401, Springer, 2005, 257-265. SJR:0.334, ISI IF:0.402, <u>Линк</u>1, <u>link2</u>

In this work we consider the rendering equation derived from the illumination model called Cook-Torrance model. A Monte Carlo (MC) estimator for numerical treatment of this equation, which is the Fredholm integral equation of second kind, is constructed and studied. An aprior estimate of the dispersion of the constructed MC estimator was obtained.

 Atanassov, E., Karaivanova, A., Gurov, T., Ivanovska, S., Durchova, M., Dimitrov, D.S.. Quasi-Monte Carlo integration on the grid for sensitivity studies. Earth Science Informatics, 3, 4, Springer-Verlang, 2010, DOI:10.1007/s12145-010-0069-9, 289-296. SJR:0.24, ISI IF:1.628, <u>Линк</u>

In this paper we present error and performance analysis of quasi-Monte Carlo algorithms for solving multidimensional integrals (up to 100 dimensions) on the grid using MPI. We take into account the fact that the Grid is a potentially heterogeneous computing environment, where the user does not know the specifics of the target architecture. Therefore parallel algorithms should be able to adapt to this heterogeneity, providing automated load-balancing. Monte Carlo algorithms can be tailored to such environments, provided parallel pseudorandom number generators are available. The use of quasi-Monte Carlo algorithms depends on the functionality of the corresponding packages for generating pseudorandom or quasirandom numbers. We propose efficient parallel implementation of the Sobol sequence for a grid environment and we demonstrate numerical experiments on a heterogeneous grid. To achieve high parallel efficiency we use a newly developed special grid service called Job Track Service which provides efficient management of available computing resources through reservations.

 Nedjalkov, M., Gurov, T., Kosina, H., Vasileska, D., Palankovski, V.. Femtosecond Evolution of Spatially Inhomogeneous Carrier Excitations Part I: Kinetic Approach. LNCS, Vol. 3743, Springer, 2006, DOI:10.1007/11666806_15, 149-153. SJR:0.317, <u>Линк</u>

The ultrafast evolution of optically excited carriers which propagate in a quantum wire and interact with three dimensional phonons is investigated. The equation, relevant to this physical problem, is derived by a first principle approach. The electron-phonon interaction is described on a quantum-kinetic level by the Levinson equation, but the evolution problem becomes inhomogeneous due to the spatial dependence of the initial condition. The initial carrier distribution is assumed Gaussian both in energy and space coordinates, an electric field can be applied along the wire. A stochastic method, described in Part II of the work, is used for solving the equation. The obtained simulation results characterize the space and energy dependence of the evolution in the zero field case. Quantum effects introduced by the early time electron-phonon interaction are analyzed.

 Gurov, T., Atanassov, E., Dimov, I. T., Palankovski, V.. Femtosecond evolution of spatially inhomogeneous carrier excitations Part II: Stochastic approach and grid implementation. Lecture Notes in Computer Science, Vol. 3743, Springer, 2006, DOI:10.1007/11666806_16, 157-163. SJR:0.34, <u>Линк</u>

We present a stochastic approach for solving the quantum-kinetic equation introduced in Part I. A Monte Carlo method based on backward time evolution of the numerical trajectories is developed. The computational complexity and the stochastic error are investigated numerically. Variance reduction techniques are applied, which demonstrate a clear advantage with respect to the approaches based on symmetry transformation. Parallel implementation is realized on a GRID infrastructure.

Научни публикации включени в групов показател Г, точки 7 и 8. (20 броя)

 Atanassov, E., Gurov, T., Karaivanova, A., Nedjalkov, M., Monte Carlo grid application for electron transport, (2006) Lecture Notes in Computer Science, 3993 LNCS - III, pp. 616-623. DOI: 10.1007/11758532_81, ISSN: 0302-9743, <u>link</u>

In this paper we present a Grid application developed for electron transport problems called SALUTE (Stochastic ALgorithms for Ultra-fast Transport in sEmiconductors). We consider a physical model of a femtosecond relaxation of optically excited electrons which interact with phonons in a one-band semiconductor. The electron-phonon interaction is switched on after a laser pulse creates an initial electron distribution. The Barker-Ferry equation is utilized as a quantum-kinetic model of the process under consideration. Two cases of this process are investigated - with and without an applied electric field. The electric field causes shift in the replicas, population of the semiclassically forbidden regions and influences the broadening and retardation of the electron distribution. The paper describes Grid implementation of these CPU-intensive algorithms. Using this application innovative results for different materials can be obtained. Here we present the first version of SALUTE which is used to obtain innovative results for GaAs materials. The results from a number of tests on MPI-enabled Grid are shown and discussed.

 Gurov, T., Atanassov, E., Ivanovska, S., A hybrid Monte Carlo method for simulation of quantum transport, (2007) Lecture Notes in Computer Science, 4310 LNCS, pp. 156-164. ISSN: 0302-9743, <u>link</u>

In this work we propose a hybrid Monte Carlo method for solving the Levinson equation. This equation describes the electron-phonon interaction on a quantum-kinetic level in a wire. The evolution problem becomes inhomogeneous due to the spatial dependence of the initial condition. The properties of the presented algorithm, such as computational complexity and accuracy, are investigated on the Grid by mixing quasi-random numbers and pseudo-random numbers. The numerical results are obtain for a physical model with GaAs material parameters in the case of zero electrical field.

 Karaivanova, A., Hongmei, C., Gurov, T., Quasi-random walks on balls using C.U.D. sequences, (2007) Lecture Notes in Computer Science, 4310 LNCS, pp. 165-172. ISSN: 0302-9743, <u>link</u>

This paper presents work on solving elliptic BVPs problems based on quasi-random walks, by using a subset of uniformly distributed sequences-completely uniformly distributed (c.u.d.) sequences. This approach is novel for solving elliptic boundary value problems. The enhanced uniformity of c.u.d. sequences leads to faster convergence. We demonstrate that c.u.d. sequences can be a viable alternative to pseudorandom numbers when solving elliptic boundary value problems. Analysis of a simple problem in this paper showed that c.u.d. sequences achieve better numerical results than pseudorandom numbers, but also have the potential to converge faster and so reduce the computational burden.

 Atanassov, E., Gurov, T., Karaivanova, A., Ultra-fast semiconductor carrier transport simulation on the grid, (2008) Lecture Notes in Computer Science, 4818 LNCS, pp. 461-469. DOI: 10.1007/978-3-540-78827-0_52, ISSN: 0302-9743, <u>link</u>

We consider the problem of computer simulation of ultra-fast semiconductor carrier transport. The mathematical description of this problem includes quantum kinetic equations whose approximate solving is a computationally very intensive problem. In order to reduce the computational cost we use recently developed Monte Carlo methods as a numerical approach. We study intra-collision field effect, i.e. effective change of phonon energy, which depends on the field direction and the evolution time. In order to obtain results for different evolution times in a reasonable time-frame, we implement simulation on the computational grid. We split the task into thousands of subtasks (jobs) which are sent to different grid sites to be executed. In this paper we present new results for inhomogeneous case in the presence of electric field, and we describe our grid implementation scheme.

 Karaivanova, A., Atanassov, E., Gurov, T., Stevanovic, R., Skala, K., Variance Reduction MCMs with Application in Environmental Studies: Sensitivity Analysis, (2008) AIP Conference Proceedings, 1067 (1), pp. 549-558. DOI: 10.1063/1.3030829, ISSN: 0094-243X, <u>link</u>

This paper studies generator sensitivity of some variance reduction Monte Carlo methods (MCMs) with acceptance-rejection for approximate calculation of multiple integrals. This investigation is important basis for the development of the grid application. Monte Carlo Sensitivity Analysis for Environmental Systems in the framework of the SEE-GRID-SCI project.

Monte Carlo are among the most widely used methods in real simulations. These methods can be considered as methods for computing an integral in the unit cube of an appropriate dimension, called the constructive dimensionality of the method.

Since its worst-case convergence rate of $O(N^{-1/2})$ does not depend on the dimension of the integral, Monte Carlo is sometimes the only viable method for a wide range of high-dimensional problems. Many studies show that the outcome of the simulation may be sensitive to the random generators being used, which means that obtaining unbiased estimates requires careful selection of the random generators. The random number generators based on physical events present an important option in this regard.

In this paper we study the sensitivity of several variance reduction Monte Carlo methods: importance sampling, smoothed importance sampling, weighted uniform sampling and crude Monte Carlo, to different type of generators: Quantum Random Bit Generator, pseudorandom generators and quasi-random sequences. Extensive numerical tests of several test integrals are presented.

 Atanassov, E., Dimitrov, D.Sl., Gurov, T., SALUTE grid application using messageoriented middleware, (2009) AIP Conference Proceedings, 1186, pp. 183-191. DOI: 10.1063/1.3265328, ISSN: 0094-243X, <u>link</u>

Stochastic ALgorithms for Ultra-fast Transport in sEmiconductors (SALUTE) is a grid application developed for solving various computationally intensive problems which describe ultra-fast carrier transport in semiconductors. SALUTE studies memory and quantum effects during the relaxation process due to electronphonon interaction in one-band semiconductors or quantum wires. Formally, SALUTE integrates a set of novel Monte Carlo, quasi-Monte Carlo and hybrid algorithms for solving various computationally intensive problems which describe the femtosecond relaxation process of optically excited carriers in one-band semiconductors or quantum wires.

In this paper we present application-specific job submission and reservation management tool named a Job Track Server (JTS). It is developed using Message-Oriented middleware to implement robust, versatile job submission and tracing mechanism, which can be tailored to application specific failover and quality of service requirements. Experience from using the JTS for submission of SALUTE jobs is presented.

 Schwaha, P., Cervenka, J., Nedjalkov, M., Gurov, T., Arsov, G., Misev, A., Zoric, A., Ilic, S., Computational electronics on GRID: A mixed mode carrier transport model, (2009) AIP Conference Proceedings, 1186, pp. 206-214. DOI: 10.1063/1.3265331, ISSN: 0094-243X, <u>link</u>

The nano-era of semiconductor electronics introduces the necessity of simulation methods which describe the electron transport in ultra-small devices in a mixed mode where quantumcoherent processes are considered along with the de-coherence processes of scattering. The latter can be conveniently described in the Wigner picture of quantum mechanics, however the coherent counterpart gives rise to heavy numerical problems. We propose a scheme which combines the advantages of the Wigner function with the Green function picture which is numerically efficient in coherent cases. An equation accounting for the scattering corrections to the coherent Wigner function is derived theoretically and a Monte Carlo algorithm for calculating these corrections is developed and implemented. The implementation is deployed on the SEE-GRID infrastructure to facilitate the swift acquisition of results. Simulation results are presented as a final point.

 14. Atanassov, E., Karaivanova, A., Gurov T., Ivanovska, S., Durchova, M., Using Sobol Sequence in Grid Environment. Proceeding of 32nd International Convention MIPRO/GVS 2009, 1, 2009, ISBN:978-953-233-044-1, 290-294, без SJR, индексирано в WoS или Scopus <u>Линк</u>

In this paper we present error and performance analysis of quasi-Monte Carlo algorithms with variance reduction, for solving multidimensional integrals on the grid using Sobol sequence. We take into account the fact that the Grid is a potentially heterogeneous computing environment, where the user does not know the specifics of the target architecture.

Therefore parallel algorithms should be able to adapt to this heterogeneity, providing automated load-balancing. Monte Carlo algorithms can be tailored to such environments, provided parallel pseudorandom number generators are available. The use of quasi-Monte Carlo algorithms poses more difficulties. In both cases the efficient implementation of the algorithms depends on the functionality of the corresponding packages for generating pseudorandom or quasi-random numbers. We propose efficient parallel implementation of the Sobol sequence for a grid environment and we demonstrate numerical experiments on a heterogeneous grid.

15. Syrakov, D., Prodanova, M., Ganev, K., Miloshev, N., Atanassov, E., Gurov, T., Karaivanova, A.. The grid computing – Powerful tool for Multi-Scale Atmospheric Composition Modelling. 9th International Multidicsciplinary Scientific Geoconference and EXPO - Modern Management of Mine Producing, Geology and Environmental Protection, SGEM 2009, 2, Surveying Geology & Mining Ecology Management (SGEM), 2009, ISBN:978-954918181-4, 365-372, **без SJR** – индексирано в WoS или Scopus <u>Линк</u>

Comprehensive atmospheric composition studies require multi-scale numerical experiments to be carried out, which to clarify to some extend different scale processes interaction, but also to further specify requirements for input data (emissions, boundary conditions, large scale forcing). Model interfaces from synoptic trough meso- to local scale have to be tailored. Shortly speaking, extensive sensitivity studies have to be carried out, tailoring the model set-up and parameters - a possible forerunner of single model ensemble forecasts. Performing extensive simulations of this kind with up to date highly sophisticated numerical models obviously requires computer resources of the order of magnitude of those provided by the so-called supercomputers. Using supercomputers, however, is rather expensive and far beyond what most of the research groups can afford. Luckily an alternative technology - the grid computing, is recently very intensively developing, which makes it already quite relevant to formulating and solving problems absolutely unthinkable several years ago. Some examples of environmental problems which are recently developed/tested/treated as grid applications are given in the present paper

 Gurov, T., Ivanovska, S., Karaivanova, A., Manev, N., Monte Carlo methods using new class of congruential generators, (2012) Advances in Intelligent and Soft Computing, 150 AISC, pp. 257-267. DOI: 10.1007/978-3-642-28664-3_24, ISSN: 1867-5662, <u>link</u>

In this paper we propose a new class of congruential pseudo random number generator based on sequences generating permutations. These sequences have been developed for other applications but our analysis and experiments show that they are appropriate for approximation of multiple integrals and integral equations.

 Karaivanova, A., Atanassov, E., Gurov, T., Monte Carlo simulation of ultrafast carrier transport: Scalability study, (2013) Procedia Computer Science, 18, pp. 2298-2306. DOI: 10.1016/j.procs.2013.05.401, ISSN: 1877-0509, <u>link</u> In this work we consider Monte Carlo methods and algorithms for solving quantum-kinetic integral equations which describe the electron transport in semiconductors. Here we study the scalability of the presented algorithms using HPC resources in South-Eastern Europe. Numerical results for parallel efficiency and computational cost are also presented. In addition we discuss the coordinated use of heterogeneous HPC resources from one and the same application in order to achieve a good performance.

 Karaivanova, A., Ivanovska, S., Gurov, T., Monte Carlo method for density reconstruction based on insufficient data, (2015) Procedia Computer Science, 51 (1), pp. 1782-1790. DOI: 10.1016/j.procs.2015.05.390, ISSN: 1877-0509, <u>link</u>

In this work we consider the problem of reconstruction of unknown density based on a given sample. We present a method for density reconstruction which includes B-spline approximation, least squares method and Monte Carlo method for computing integrals. The error analysis is provided. The method is compared numerically with other statistical methods for density estimation and shows very promising results.

 Atanassov, E., Gurov, T., Karaivanova, A., Parallel grid applications, (2015) Grid Computing: Techniques and Future Prospects, pp. 129-155. ISBN: 978-163482326-5;978-163117704-0, <u>link</u>

In this chapter we discuss the development of parallel applications using the Grid environment. Two alternative strategies are widely used: (i) executing large number of batch jobs in a coordinated way, and, (ii) executing parallel jobs (using MPI and/or OpenMP). The chapter starts with a short description of the parallel computing and MPI standard, then goes on to present and discuss various parallelization strategies in Grid environment, including integration of MPI in the Grid middleware. A special attention has been given to tools which speed-up the job execution, such as a service developed by us called JTS (Job Track Service), as well as some techniques for the map-reduce processing model. Finally, the Grid application SALUTE (Stochastic Algorithms for Ultrafast Electron Transport) is presented as a case study, in order to illustrate some practical aspects of the above topics, covering the Grid implementation schemes with and without MPI, graphical interface, use of reservation services, visualization and scalability results. Since in practice a large part of the computational resources, interconnected in Grids, is used for various types of Monte Carlo simulations, many of the tools and services that we describe are geared towards such problems. In order to support the execution of such computations, researchers use frameworks, libraries and services for launching, monitoring and output gathering. In our scientific research we have great experience with using Monte Carlo Methods in various applied areas. Our experience with the successfully used tools and techniques is also presented in this chapter.

20. Radenski, A., Gurov, T., Kaloyanova, K., Kirov, N., Nisheva, M., Stanchev, P., Stoimenova, E., Big data techniques, systems, applications, and platforms: Case studies from academia, (2016) Proceedings of the 2016 Federated Conference on Computer Science and Information Systems, FedCSIS 2016, pp. 883-888. DOI: 10.15439/2016F91, ISBN:978-8-3608-1090-3 ISSN: 2300-5963, <u>link</u> Big data is a broad term with numerous dimensions, most notably: big data characteristics, techniques, software systems, application domains, computing platforms, and big data milieu (industry, government, and academia). In this paper we briefly introduce fundamental big data characteristics and then present seven case studies of big data techniques, systems, applications, and platforms, as seen from academic perspective (industry and government perspectives are not subject of this publication). While we feel that it is difficult, if at all possible, to encapsulate all of the important big data dimensions in a strict and uniform, yet comprehensible language, we believe that a set of diverse case studies-like the one that is offered in this paper a set that spreads over the principal big data dimensions can indeed be beneficial to the broad big data community by helping experts in one realm to better understand currents trends in the other realms.

 Atanassov, E., Gurov, T., Karaivanova, A., Ivanovska, S., Durchova, M., Dimitrov, D., On the parallelization approaches for Intel MIC architecture, (2016) AIP Conference Proceedings, 1773. DOI: 10.1063/1.4964983, ISSN: 0094-243X, <u>link</u>

The Intel MIC architecture is one of the main processor architectures used for the production of computational accelerators. Increasing energy and cost-efficiency of accelerators is one important option for building new HPC systems. However, the effective use of accelerators requires careful optimization on all stages of the algorithm and use of appropriate parallelization approaches. In the domain of statistical methods the quasi-Monte Carlo methods present distinct challenges when thousands of computational cores are to be involved in a computation. In this paper we describe in detail and study the performance of algorithms for generating some popular low-discrepancy sequences, aimed at devices with Intel MIC architecture. By leveraging the powerful vector instructions of the Intel MIC architecture to process many coordinates of the sequences in parallel, we obtain fast implementations that can be plugged-in in any parallel quasi-Monte Carlo computation. We present extensive numerical and timing results that demonstrate the benefit of our algorithms and their parallel efficiency. The effects of using hyperthreading are also studied. The generation routines are provided under the GPL.

22. Gurov, T., Karaivanova, A., Alexandrov, V., Energy study of Monte Carlo and Quasi-Monte Carlo algorithms for solving integral equations, (2016) Procedia Computer Science, 80, pp. 1897-1905. DOI: 10.1016/j.procs.2016.05.492, ISSN:1877-0509, link

In the past few years the development of exascale computing technology necessitated to obtain an estimate for the energy consumption when large-scale problems are solved with different high-performance computing (HPC) systems. In this paper we study the energy efficiency of a class of Monte Carlo (MC) and Quasi-Monte Carlo (QMC) algorithms for a given integral equation using hybrid HPC systems. The algorithms are applied to solve quantum kinetic integral equations describing ultra-fast transport in quantum wire. We compare the energy performance of the algorithms using a GPU-based computer platform and CPU-based computer platform both with and without hyper-threading (HT) technology. We use SPRNG library and CURAND generator to produce parallel pseudo-random (PPR) sequences for the MC algorithms on CPU-based and GPU-based platforms, respectively. For our QMC algorithms Sobol and Halton sequences are used to produce parallel quasi-random (PQR) sequences. We compare the obtained results of the tested algorithms with respect to the given energy metric. The results of our study demonstrate the importance of taking into account not only scalability of the HPC intensive algorithms but also their energy efficiency

They also show the need for further optimisation of the QMC algorithms when GPU-based computing platforms are used.

Gurov, T., Atanassov, E., Karaivanova, A., Serbezov, R., Spassov, N., Statistical Estimation of Brown Bears (Ursus arctos L.) Population in the Rhodope Mountains, (2017) Procedia Computer Science, 108, pp. 2028-2037. DOI: 10.1016/j.procs.2017.05.272, ISSN: 1877-0509, <u>link</u>

The brown bear (Ursus arctos L.) is the most widespread bear in the world. It can be found across Europe, Asia and North America in habitats ranging from forests to dry deserts and tundra. One of the best natural habitats of brown bears (Ursus arctos L.) in Europe are located in Bulgaria. They are situated in the mountain massifs: The Rhodopes, Balkan Mountains, Rila, Pirin, and Vitosha. The species is a strictly protected and the Nature protection act declared areas for conservation of its habitats. That is why it is important to estimate the population size of brown bears and how this population is changed in the country during the years. In this work we study the population of brown bears in the Rhodope Mountains, using statistical data received from the National monitorings which were carried out in autumn 2011 and 2012. The observed data during the National monitorings are incomplete and contains some uncertainties. Here we suggest some approaches to resolve this problem and obtain a satisfactory estimate of the brown bear population in The Rhodopes. The suggested approaches can be applied to estimate the population of the species in the other mountain massifs.

24. Karaivanova, A., Alexandrov, V., **Gurov, T.**, Ivanovska, S., On the Monte Carlo matrix computations on Intel MIC architecture, (2017) Cybernetics and Information Technologies, 17 (5), pp. 49-59. DOI: 10.1515/cait-2017-0054, ISSN: 1311-9702, <u>link</u>

The tightened energy requirements when designing state-of-the-art high performance computing systems lead to the increased use of computational accelerators. Intel introduced the Many Integrated Core (MIC) architecture for their line of accelerators and successfully competes with NVIDIA on basis of price/performance and ease of development. Although some codes may be ported successfully to Intel MIC architecture without significant modifications, in order to achieve optimal performance one has to make the best use of the vector processing capabilities of the architecture. In this work we present our implementation of Quasi-Monte Carlo methods for matrix computations specifically optimised for the Intel Xeon Phi accelerators. To achieve optimal parallel efficiency we make use of both MPI and OpenMP.

25. Atanassov, E., Gurov, T., Ivanovska, S., Karaivanova, A., Simchev, T., On the parallel implementation of quasi-monte carlo algorithms, (2018) Lecture Notes in Computer Science, 10665 LNCS, pp. 258-265. DOI: 10.1007/978-3-319-73441-5_27, ISSN: 0302-9743, <u>link</u>

The quasi-Monte Carlo algorithms utilize deterministic low-discrepancy sequences in order to increase the rate of convergence of stochastic simulation algorithms. Such kinds of algorithms are widely applicable and consume large share of the computational time on advanced HPC systems. The recent advances in HPC are increasingly rely on the use of accelerators and other similar devices that improve the energy efficiency and offer better performance for certain type of computations. The Xeon Phi coprocessors combine efficient vector floating point computations with familiar operational and development environment. One potentially difficult part of the conversion of a Monte Carlo algorithm into a quasi-Monte Carlo one is the generation of the low-discrepancy sequences. On such specialized equipment as the Xeon Phi, the value of memory increases due to the presence of a large number of computational cores. In order to allow quasi-Monte Carlo algorithms to make use of hybrid OpenMP+MPI programming, we implemented generation routines that save both memory space and memory bandwidth, with the aim to widen the applicability of quasi-Monte Carlo algorithms in environments with an extremely large number of computational elements. We present our implementation and compare it with regular Monte Carlo using a popular pseudorandom number generator, demonstrating the applicability and advantages of our approach.

26. Alexandrov, V., Davila, D., Esquivel-Flores, O., Karaivanova, A., Gurov, T., Atanassov, E., On monte carlo and quasi-monte carlo for matrix computations, (2018) Lecture Notes in Computer Science, 10665 LNCS, pp. 249-257. DOI: 10.1007/978-3-319-73441-5_26, ISSN: 0302-9743, <u>link</u>

This paper focuses on minimizing further the communications in Monte Carlo methods for Linear Algebra and thus improving the overall performance. The focus is on producing set of small number of covering Markov chains which are much longer that the usually produced ones. This approach allows a very efficient communication pattern that enables to transmit the sampled portion of the matrix in parallel case. The approach is further applied to quasi-Monte Carlo. A comparison of the efficiency of the new approach in case of Sparse Approximate Matrix Inversion and hybrid Monte Carlo and quasi-Monte Carlo methods for solving Systems of Linear Algebraic Equations is carried out. Experimental results showing the efficiency of our approach on a set of test matrices are presented. The numerical experiments have been executed on the MareNostrum III supercomputer at the Barcelona Supercomputing Center (BSC) and on the Avitohol supercomputer at the Institute of Information and Communication Technologies (IICT).