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Lodz University of Technology

Dedicated parallel machines - a breakthrough in computation

ARUZ-Workshop 2016

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BOOK OF ABSTRACTS

Lodz University of Technology, Technopark Lodz

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Book of abstracts & programme

Preface

The Workshop is organized by Lodz University of Technology and Technopark Lodz in Lodz (Poland) on 01-03.12.2016 under the auspices of Rector of Lodz University of Technology. The main topic is devoted to dedicated machines applied to computation, modeling and data processing. Scope of the workshop covers simulation and modeling, dedicated machines and dedicated electronic solutions.

The central idea is dedicated to different possible applications of massively-parallel simulator ARUZ -Analyzer of Real Complex Systems (pol. Analizator Rzeczywistych Układów Złożonych), which is a core of the Laboratory of Molecular Simulation, perhaps the most unique unit of the BioNanoPark project laboratories in Technopark. This part of BioNanoPark was elaborated at Lodz University of Technology, a shareholder of Technopark Lodz, as a part of the European Centre of Bio- and Nanotechnology in Lodz. ARUZ was constructed in Technopark Lodz with currently implemented Dynamic Lattice Liquid (DLL) cellular automaton algorithm. ARUZ consist of 27 000 FPGA (Field Programmable Gate Arrays) implemented in one structure interconnected in dense three-dimensional network. This makes it a dedicated machine optimized for three dimensional simulations of systems containing theoretically up to few millions of elements (united atoms representing molecules, atoms, groups of atoms) in long time scales. Implemented algorithm enables dynamic simulation of chemical and physical phenomenon in liquid and soft matter systems, like polymerization, diffusion, self-organization, aggregation, confined space effect and others. The FPGA-based design makes ARUZ a good ground for implementation of other parallel algorithms, where local interactions between many simple elements are crucial.

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We kindly acknowledge Dr. Agnieszka Ślązak and Dr. Marcin Kozanecki for help in organization.

Workshop programme

Thursday 01.12.2016 (at Technopark Lodz)

09.15 – 10.00 – Registration

10.00 – 10.20 – Opening by Scientific Committee Chairmen and Representatives of Technopark and TUL

10.20 – 10.40 – **Jacek Ulański, Andrzej Napieralski, Przemysław Panek** – *The Origin of ARUZ*

10.40 – 11.20 – **Rafał Kiełbik, Grzegorz Jabłoński, Piotr Amrozik, Zbigniew Mudza, Joanna Kupis** – *ARUZ - the unique massively parallel FPGA-based system*

11.20 – 11.40 – Coffee break

11.40 – 12.40 – Visiting of ARUZ

12.40 – 14.00 – Lunch break

14.00 – 14.40 – **Krzysztof Hałagan** – *Modelling of complex liquids with cooperative dynamics using ARUZ*

14.40 – 15.20 – **Agnieszka Dybała-Defratyka** – *Current Challenges and Achievements of Computational Chemistry*

15.20 – 16.00 – **Paweł Russek** – *FPGA-enhanced algorithms for browsing and searching in high performance and energy-efficient applications*

16.00 – 16.20 – Coffee break

17.00 – 17.40 – **Zbigniew Koza** – *Graphics processors as general-purpose computing units*

17.40 – 18.20 – **Andrzej Sikorski** – *Structure of polymers determined from advanced Monte Carlo simulations: Replica Exchange and parallel computing*

18.30 – Shuttle bus to hotel and dinner at 20.00

Friday 02.12.2016 (at CSK UL)

08.00 – 09.30 – Breakfast

09.30 – 10.10 – **Adam Skorek** – *Canadian Approach to the High Performance Computing in Science and Engineering*

10.10 – 10.50 – **Marcin Szymonek/Tamas Barbarics** – *Xilinx All Programmable FPGA and SoC solutions: overview and applications*

10.50 – 11.10 – Coffee break

11.10 – 11.50 – **Jeremiasz Jeszka** – *Simulations of Living Polymerization in Complex Polymer Systems by DLL Method*

11.50 – 12.30 – **Peter Cifra** – *Simulation of linear and ring DNA in nanochannels*

12.30 – 14.00 – Lunch break

14.00 – 14.40 – **Robert Boesnecker** – *An internal view to ARUZ from outside*

14.40 – 15.20 – **Andrzej Eilmes** – *Efficiency of molecular modeling on Graphics Processing Units – an example from physical chemistry of electrolytes*

15.20 – 16.00 – **Michał Banaszak** – *Florian polymer physics of the 21st century - a concept and some useful examples*

16.00 – 16.20 – Coffee break

16.20 – 18.00 – Poster session

18.00 – 19.00 – Discussion panel (Chairman Kazimierz Wiatr)

19.00 – Official dinner + End of workshop

Saturday 03.12.2016

8.00 – 09.30 – Breakfast

10.30 – Shuttle bus to Lodz center

LECTURES

ARUZ - the unique massively parallel FPGA-based system

Rafał Kiełbik, Grzegorz Jabłoński, Piotr Amrozik, Zbigniew Mudza, Joanna Kupis

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Simulations of physical phenomena at the molecular level require plenty of molecules to be considered in parallel. Attempts to accelerate such simulations using multi-core supercomputers suffer from the interconnection limitations - each molecule must exchange relatively small portions of data but with multiple recipients - all the nearest neighbors, in many directions, with lowest possible latency. Unfortunately, supercomputers are equipped with high-bandwidth buses and advanced communication protocols that are more suitable for big data packages being exchanged among limited number of centralized data sources and destinations. Furthermore, processor cores of supercomputers are often much too complex, thus also too power consuming to emulate a single molecule efficiently.

ARUZ (in Polish.: Analizator Rzeczywistych Układów Złożonych - Analyzer of Real Complex Systems) is a simulator designed and developed in order to overcome the problems mentioned above. It is a scalable, fully parallel data processing system equipped with low-latency communication channels, dedicated to simulations based on modeling emulation of interactions among huge amount of relatively simple elements. These elements can represent molecules in simulations of physical phenomena at the molecular level but they can also correspond to any simple components

of various complex systems, allowing simulations of different phenomena at the required level.

Presentation is focused on the most important technical aspects of ARUZ construction. Its main building blocks will be depicted and the way they operate and interact will be explained.

Modelling of complex liquids with cooperative dynamics using ARUZ

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Modelling and simulation of complex liquids like polymer systems or porous media is becoming more and more important field of research. Especially difficult is simulation of dynamic behaviour and diffusion in this kind of systems. This challenging area plays important role in prediction and explanation of experimentally observed phenomenon. The unique approach was proposed by Prof. Pakula – called Dynamic Lattice Liquid (DLL) [1]. This Monte Carlo model is based on the assumption that molecular diffusion steps are realized as a cooperative motion of coarse-grained elements.

DLL was already successfully applied for various non-equilibrium physical and chemical problems in polymer science, like linear [2] and cyclic polymer chains dynamics [3], gelation process [4], solvent dynamics in the neighbourhood of brushed polymer chains [5], phase separation kinetics [6], diffusion in complex environments [7]. The unique dynamic properties and parallel nature of DLL gave basis for the idea of massively-parallel simulator – ARUZ (Analyzer of Real Complex Systems). It can be used in a number of research fields, including macromolecular chemistry, simulations of systems with bio-like macromolecules, condensed and soft matter physics, etc. The basic DLL algorithm implemented on ARUZ was extended with different mechanisms allowing simulations far beyond just a stochastic diffusive motion. This mechanisms can take into account various phenomena, like chemical reactions of different orders, covalent bond creation and breaking, local non-covalent interactions, and also scalar and vector fields for spatial

variation of these quantities. User-friendly interface allows to simply set up simulation experiment by specifying its parameters used mainly as a probability tests criteria. Other details like boundary conditions for 3D simulation box can also be defined.

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[5] M. Kozanecki, K. Halagan, J. Saramak, K. Matyjaszewski, *Soft Matter* **12**, 5493 (2016); J. Saramak, K. Halagan, M. Kozanecki, P. Polanowski, *J. Mol. Model.* **20**, 2529 (2014).
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Current Challenges and Achievements of Computational Chemistry

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Over the past decades scientific community could observe an amazing boom in the development of computational chemistry methods. Calculations at classical and quantum mechanical levels have been accelerated due to various approaches such as fast scaling methods as well as graphical processing unit (GPU) architectures. The sizes of the systems which can be simulated have increased during recent years allowing to treat more atoms at a quantum level on the one hand and pushing the limits of biological systems at classical level on the other one. Although the computational treatment of chemical systems is already well established and independent research field there are still aspects calling for attention and increased activity of its experts. In order to pinpoint some grand recent challenges and achievements selected notable reported examples of calculations will be presented and discussed.

FPGA-enhanced algorithms for browsing and searching in high performance and energy-efficient applications

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Browsing and searching constitute important pillars of contemporary computing systems. In the era of Internet, the volume of information stored in the data repositories grows rapidly and that implies the need for its efficient processing. That efficiency must be measured not only in the high speed but in the low energy consumption as well. With the growing demand for the high-quality processing in a specific algorithm domain, the applicability of custom processing architectures usually appears. The custom architectures always offer the best performance and energy efficiency, and the FPGAs are most flexible, software-like programmable technology for custom computing with the dedicated machines today.

Unfortunately, browsing and searching are not compute-intensive problems that are commonly recognized as the most adequate for custom computing acceleration. In the presentation, some ideas and results will be given to demonstrate that the data-intensive browsing and searching can be successfully enhanced in the hybrid nodes, where CPU is accompanied by the FPGA structure.

Graphics processors as general-purpose computing units

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Massively parallel computations on graphics processing units (GPUs) is an emerging technology that has already seriously affected the high-performance computing industry. We show how GPUs attempt to cope with some fundamental technological barriers that for about a decade now have hindered the progress in the efficiency of "ordinary" computers. We present the most important features of modern graphics cards that make them an attractive platform for physics simulations and numerics, as well as their weaknesses, which have prevented their wide adoption in the community. We also report some of the recent achievements of our faculty group in applying this technology to scientific problems: efficient low-level implementations of some basic numerical algorithms [1-3] and the porting of complex algorithms to the new software and hardware platform [4-5].

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[2] J. L. Greathouse, K. Knox, J. Poła, K. Varaganti, M. Daga, *clSPARSE: A Vendor-Optimized Open-Source Sparse BLAS Library*, IWOCL '16 Proceedings of the 4th International Workshop on OpenCL, a. 7, 2016.

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[4] T. Tomczak, K. Zadarnowska, Z. Koza, M. Matyka, Ł. Mirosław, *Acceleration of iterative Navier-Stokes solvers on graphics processing units,* Int. J. Comput. Fluid Dynamics 27, 201-209, 2013.

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Structure of polymers determined from advanced Monte Carlo simulations: Replica Exchange and parallel computing

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The structure of chains in polymer systems was a subject of computational study. A Monte Carlo method was chosen a simulation tool. Because of size of such systems and their complexity only coarse-grained model are makes the simulations feasible. The Bond Fluctuation Model of polymer chains was presented against other lattice and off-lattice models [2]. The applicability of the Replica Exchange algorithm applied to polymer systems [1] was shown and discussed. The algorithms for polymer simulations to parallel computing were analyzed and evaluated [3].

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Canadian Approach to the High Performance Computing in Science and Engineering

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Canadian experience in High Performance Computing [1] can be very useful for any country which starts implementation or has already some supercomputers infrastructures in use. In fact, Canadian supercomputers are rated in top500 list for many years [2] and all performance, storage, access, commercial software and financial issues was pragmatically approached with success but also with some problems solved or not. In this presentation, Compute Canada with regional organizations ACENET, Calcul Québec, Compute Ontario and WestGrid will be explored with a special invitation to an academic cooperation in the use of the advanced research computing (ARC), storage and software solutions. More than 200 experts employed by 37 Canadian partner universities and research institutions provide currently direct support to the Compute Canada infrastructure users. How to access this infrastructure from Poland and how to share common resources? – available opportunities will be shown and explain with details, assuming than an appropriate online access will be provided in the conference room. In particular, a distance use of some commercial software as MATLAB, COMSOL and ANSYS will be related to the licensing from Canadian Microsystems Corporation [3]. Finally, implementation of the FDTD software in the Compute Canada parallel computing environment will be shown as an opportunity for cooperative open and/or commercial research activities, and that from the worldwide perspective [4], [5].

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[5] http://ab-initio.mit.edu/wiki/index.php/Meep, 28-11-2016.

Xilinx All Programmable FPGA and SoC solutions: overview and applications

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On behalf of Avnet Silica – the worldwide leader in distribution of electronic components and authorized technological partner of Xilinx Inc., we would like to introduce an audience to comprehensive portfolio of FPGA/SoC devices as well as auxiliary software solutions.

Xilinx offers a comprehensive multi-node portfolio of FPGA's to address requirements across a wide set of applications. Whether you are designing a state-of-the art, high-performance networking application requiring the highest capacity and performance, or looking for a low-cost, small footprint FPGA to take your software-defined technology to the next level, Xilinx All Programmable FPGAs and 3D ICs provide you with system integration while optimizing for performance/watt.

Xilinx's All Programmable SoC portfolio integrates the software programmability of a processor with the hardware programmability of an FPGA, providing you with unrivaled levels of system performance, flexibility, and scalability. SoC portfolio gives your designs overall system benefits of power reduction and lower cost with fast time to market. Unlike traditional SoC processing solutions, the flexible programmable logic provides you with optimization and differentiation, allowing you to add the peripherals and accelerators you need to adapt to a broad base of applications.

Simulations of Living Polymerization in Complex Polymer Systems by DLL Method

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Complex polymers systems such as stars, brushes nanogels ect. are extensively studied in recent years and find various practical applications. Atom transfer radical polymerization (ATRP) method makes possible precise control of the polymerization process and obtaining such materials in a convenient, one-pot method. In the first approximation it can be considered as living polymerization (no termination). During the polymerization of complex macromolecules diffusion constants, molecular weights, local polymer density and polymer structure change dramatically so simulation method which is able to take changing local diffusion of the reagents into account. Dynamic lattice liquid (DLL) method of Monte Carlo simulation proposed by T. Pakula based on analysis of cooperative movements [1] is therefore most suitable in such cases. It consists in simultaneous moving of all elements in the simulation box which are able to move at the moment i.e. their move does not violate excluded volume or chain integrity condition. This method is also suitable to perform simulations on dedicated machine and is implemented in ARUZ.

In this lecture we present some results of DLL simulations of ATRP synthesis of complex polymer systems involving star polymers, gels and polymer brushes. Stars and gels are obtained by suitable copolymerization of a vinyl monomer and bifunctional crosslinker. Two methods of star preparations were simulated: (i) arm-first, where the linear arms are grown first and then crosslinker is added to form star cores and (ii) core-first,

where crosslinker forms cores at the beginning. In particular they show importance of dilution and full conversion of the crosslinker for the average number of arms of the obtained stars and possible gelation. Simulations of gelation provide evidence of the importance of intramolecular cyclization for the position of gelation point. The simulations of synthesis of polymer brushes i.e. sets of polymer chains with one end grafted to an impenetrable wall show importance of the grafting density and polymerization rate for the properties of the obtained brushes. The results are in good agreement with experimental data and can be used as a guidelines in the experiment.

Acknowledgement: The authors gratefully acknowledge the financial support of this research by the National Science Centre of Poland, grant UMO-2014/14/A/ST5/00204.

[1] P. Polanowski and T.Pakula, *Journal of Chemical Physics* 2002, **117**, 4022-4029.

Simulation of linear and ring DNA in nanochannels

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Problems in the field of polymers, or generally of soft matter, due to complexity of systems involved and a broad span of typical distances and characteristic times require a strong computational power to handle. To investigate a generic behavior of whole systems often coarse-grained models are used. This study represents such approach in the next generation DNA sequencing that is quick and cheap compared to classical Sanger method. The method uses single molecule real time sequencing, can use large strides along the whole sequence and thus allows for mapping of organization and repeat of sequences, in order to obtained contextual information that is often lost in fragmentation. The connection between mapping and sequencing is analogous to exploring Google maps with zoom in/out function. Mapping is obtained with fluorescent microscopy images of DNA linearized in nanochannels in the form of a barcode, i.e. term ”DNA barcoding” [1].

We investigate suggested advantageous analysis in the linearization experiments with DNA macromolecules confined in a stripe-like channel using Monte Carlo and molecular dynamics simulations [2, 3]. The enhanced chain extension in a stripe that is due to significant excluded volume interactions between monomers in two dimensions weakens on transition to experimentally feasible slit-like channel. Based on the chain extension-confinement strength dependence and on the structure factor behavior for the chain in stripe we infer the excluded volume regime typical for two-dimensional systems. On transition to the slab geometry, the advantageous

chain extension decreases and the Gaussian regime is observed for not very long semi-flexible chains. The evidence for pseudo-ideality in confined chains is based on indicators such as the chain extension curves, variation of the extension with the persistence length or the structure factor. The slab behavior is observed when the stripe (originally of monomer thickness) reaches the thickness larger than cca 10nm in the third dimension. This maximum height of the slab to retain the advantage of the stripe is very low and this have implication for DNA linearization experiments [2]. The presented analysis, however, has a broader relevance for confined polymers.

Comparison of ring and linear macromolecule showed a stronger relative chain extension of ring relative to the linear chain what is in accord with enhanced self-avoidance in channel-confined ring [3]. As for the linear chains we present details on transition between the stripe and slab geometry also for rings.

Support from Slovak R&D Agency (SRDA-0323-15) and VEGA 2/0098/16, VEGA 2/0055/16 is acknowledged.

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An internal view to ARUZ from outside

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The scope of the presentation is to unleash the calculating power of the ARUZ cluster. Two proposals are given. In a first proposal the fixpoint calculation power is discussed. The FPGA itself provides some highly effective means to implement a 18 bits by 25 bits parallel multiply/accumulator hardware with a maximum of about 900 GMAC/s. This large amount of digital signal processing power enables the ARUZ to process a massive amount of payload data. In contrast we find a data input speed to the cluster of 2 x 125 MByte/s only. This contradiction leads to the conclusion, that the DSP algorithms inside the ARUZ FPGA cluster can only be fed by a small amount of realtime data input coming from the servers. The proposal given here is to use the inside calculation power to emulate "musical" instruments while the stream of input data is used to update control data within the cluster. With a maximum of about 700 DSP cores per FPGA also human voices can be synthesized.

Another feature of the cluster is, that the FPGAs are working asynchronously. Using special "reporting" signals the outputs of the FPGAs are tagged to communicate with neighbor FPGAs. Therefore a second proposal is made: use the ARUZ cluster as cryptographic machine. DES and AES algorithms are discussed shortly to propose a new 3 dimensional encryption algorithm that meets the constrains of the cluster. Based on this "Lodz encryption" algorithm a new service could be offered worldwide. Using the huge amount of logical operations and memory storage per FPGA

a highly efficient cipher algorithm can be implemented and even run in parallel streams. Governments, hospitals, and the like could use the future "Lodz Encryption Service" to save their sensitive data before storing.

[1] Xilinx ARTIX DSP Slice UG479 7Series DSP48E1 User Guide, 2016
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[3] Xilinx ARTIX AC DC ds181 Artix 7 DataSheet , 2016
[4] Xilinx ARTIX 7_Series product selection guide , 2016
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Efficiency of molecular modeling on Graphics Processing Units – an example from physical chemistry of electrolytes

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Methods of computational chemistry are invaluable tools in modeling of complex systems in physical chemistry, materials science or biochemistry, providing deeper insight into the nature of observed processes and helping to understand and to explain experiments. Their use requires quite often significant computational resources needed to apply more advanced quantum-chemical methodology, to study larger systems or to achieve longer simulation times in molecular dynamics. This constant demand for increasing computational power for molecular modeling stimulates growing interest in hardware acceleration, in particular in general purpose computing on Graphics Processing Units (GPUs).

In this work we assessed effectiveness of GPU computing on GPU partition of Prometheus - the most powerful computer cluster in the Academic Computer Centre "Cyfronet" AGH in Kraków [1]. As a test system we used electrolytes based on ionic liquids – solvents attracting recently significant scientific attention owing to their prospective applications. We will report scalability of molecular dynamics simulations using NAMD software [2] and the advantages of GPU acceleration, discussing dependence on system size and the parameterization of the force-field.

In the second part of the talk we will present applications of GPU computing to quantum-chemical calculations, including ab initio molecular dynamics, performed for sample ionic liquid in TeraChem software [3].

[1] https://kdm.cyfronet.pl/portal/Prometheus.
[2] NAMD – Scalable Molecular Dynamics, http://www.ks.uiuc.edu/Research/namd/.
[3] TeraChem, http://www.petachem.com/.

Florian polymer physics of the 21st century - a concept and some useful examples

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Flory' s lattice model of polymer blends and solutions is explored both by traditional numerical calculations and by Monte Carlo simulations which employ both Cooperative Motion Algorithm and Parallel Tempering methods. In particular, we apply this approach to "dry" ionic copolymers which exhibit an unusual phase behavior and can be used in lithium batteries and fuel cells as membranes. We also show that in triblock copolymer melts a new type entropy-driven micelles is formed which can further be used, for example, to modify the rheological properties of those melts.

POSTERS

The ARUZ Supersimulator: DBoard Embedded System

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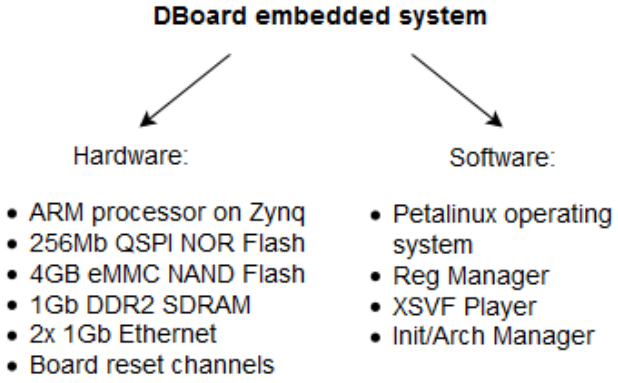
The poster presents the embedded system supervising the operation of every DBoard in the ARUZ supersimulator. It is running on the Xilinx Zynq (DMaster) and controls 8 DSlave FPGAs. It manages:

- the startup sequence,
- the firmware update,
- the bridging of on-board Ethernet ports,
- the configuration of DSlaves via JTAG interface,
- controlling and reading status of DSlaves,
- collecting and distributing simulation initialization data to DSlaves,
- collecting and transferring data generated during simulation to servers.



The embedded system is based on Petalinux OS [1] and contains a set of scripts and services written in C and C++. Initialization of computing nodes and archivization of simulation results is handled by the Init/Arch Manager service together with the low-level DMA driver. Access to control and status registers of DSlaves is provided by Reg Manager service. Configuration of DSlaves is performed via the Zynq GPIO pins and boundary scan interface using the XSVF player application. Apart from these specialized services FTP and SSH are used for control and data transfer.

In normal operation mode the embedded system boots from eMMC. However it is also possible to boot the system from the network to update the eMMC contents. The SPI flash memory containing the bootloader is write-protected to avoid accidental corruption, enabling system recovery from the control room without the need of entering ARUZ and connecting a service rig to DBoard.

[1] Xilinx; PetaLinux Tools Documentation - Reference Guide (UG1144), December 2015.

ARUZ Dedicated Software

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The user front-end access to ARUZ is possible using dedicated web browser applications. Moreover, software tools at various levels were developed to provide proper management of the entire system. One set of tools is designed for: system supervision, archiving and aggregation of output files, power management, logging hardware issues, collecting of all measurement data and handling of alarm conditions. Second is responsible for: selection of simulation variant and its parameters, input file generation, management and logging of simulation tasks, access to and some basic analysis of output files. Finally, third tool is used for: access to, visualization and logging of measurement data.

ARUZ currently implements the DLL (Dynamic Lattice Liquid) [1] cellular automaton algorithm. Examples of use of DLL in the field of dynamic processes, and non-equilibrium phenomenon in general, can be found in the literature [2,3,4]. To enable flexibility of ARUZ in different potential applications, the basic DLL algorithm was extended with different mechanisms allowing simulations far beyond just a stochastic diffusive motion. In addition to simulation initial configuration setup, every mechanism have to be parameterized by user in application. For example, setting up full thermal interactions between different molecules can involve over 500 probability values to define in extreme case. Spatial variations of probability values can also be defined.

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The ARUZ Supersimulator: Board Testing System

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The poster presents the system that has been used to test printed circuit boards constituting components of the ARUZ supersimulator. Because of the large number of boards (2880 DBoards, 20 CBoards and 1 MBoard) a special fixture and the appropriate test software, called Devstarter, have been developed for automatic initialization and test of the boards.

The boards coming from production after visual inspection were put on a specially designed test rig. Every board was labeled by the manufacturer with a unique serial number, read automatically using the barcode scanner. The test results were put into the database, allowing identification of the history of each board and assigning them unique Ethernet MAC addresses. The test sequence included:

- verification of power consumption of the board
- QSPI flash programming, including configuration of Ethernet card MAC addresses
- QSPI flash write protection
- UART test
- eMMC test and setup
- OS image download
- master FPGA (Zynq) bitstream programming
- verification of control communication connectivity

- test of Ethernet bridge (using Iperf)
- slave FPGA bitstream programming
- test of bit error rate of local communication using short loopback cables

If errors were detected, operator could repeat the test after e.g. fixing the connections or cabling mistakes as well as send the board to the manufacturer for repair.

The most frequent defect were the missing or damaged series capacitors on differential local communication links (1 Gb/s). About 10% of the boards had some issues to fix.

The test database was also very useful during ARUZ commissioning, as it contains the entire history of every board. It turned out, that many boards that caused problems during simulations have been repaired multiple times.

The difference in diffusive properties of bound and bulk water as seen by Monte Carlo simulations

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Porous polymer systems fulfilled by water or other solvents, such as hydrogels and organogels, filters, membranes and absorbers are commonly used in many various branches of human activity. Also different polymer solutions and dispersions are widely used as coating layers (paints, lacquers), glues, components of cosmetics, foods and pharmaceutics and many others. It is necessary to underline that polymers have to be characterized by averaged values because of distribution of their molecular masses, numerous conformations available for big macromolecules resulting in variation of segmental dynamics, concentration and interactions in micro-scale. For porous systems variation of pore size should be also taken under consideration. Due to that, to characterize polymer systems properly, relatively wide computational box is required for simulations. Moreover, most of these systems exhibit slowed diffusion due to significant difference in size of polymer chain and solvent molecule leading to extremely high difference in mobility of these two types of species [1]. In result polymer systems are very demanding for computational studies because of both time and size scales requirements.

Parallel algorithms may significantly reduce the calculation time, but they need special, parallel computing machines to work effectively. In the present work the problem of solvent diffusion in model solvent-polymer (water-polyvinylmethylether) solutions differing on concentration and polymer chain length is discussed. The DLL algorithm was used to distinguish

difference in diffusive properties of solvent molecules in direct neighborhood of macromolecule and in bulk. A correlation between solvent mobility and homogeneity of the solution is shown [2,3].

This work was financially supported by Polish National Science Center grant no. 2013/09/B/ST4/03010 and 2014/14/A/ST5/00204.

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A Different View of ARUZ: Systolic Array Approach

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The poster focuses on the possible extension of the ARUZ capabilities, which are for now limited to one problem only, i.e. machine is dedicated for the DLL algorithm. It is one of the greatest advantages of this supersimulator, that it is optimized for specific computations. On the other hand however it is a great waste of resources if it stays that way without any further modification and functionality extensions, especially bearing in mind, that the ARUZ machine is built to be reprogrammed and reconfigured. Thus this limitation is not due to the hardware design but to complex and cumbersome software development process. What we are trying to achieve is to simplify this complexity, making the supersimulator more adjustable to our needs. During the first phase of our research, we are trying to find algorithms, which are computationally expensive and suitable for acceleration and optimization. This is where the FPGA-based construction fits perfectly. Through its interconnection topology, the ARUZ platform is a natural candidate for implementation of systolic arrays or wavefront processors. Research on programming languages and tools for reprogrammable system of such structure has already been conducted for several years. The PARO design system [1] with its multilevel partitioning technology together with PAULA language is one example of considered approach. Another interesting tool set is Riverside Optimizing Compiler for Configurable Computing (ROCCC) [2], [3]. Here, the loop nest is transformed into a systolic array implementation, resulting in an impressive speedup of 3600 for the Smith-Waterman algorithm.

The poster presents methods for automatic systolic array generation in the context of further development of the ARUZ supersimulator.

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Developing a coarse-grained mucus model

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Mucins are large, extracellular, heavily glycosylated proteins that play a role in human immune system. Capable of polymerization and gel formation they are a selective molecular barrier that controls the cell's microenvironment and take part in signal transduction. Due to their importance mucins are a target of cancer treatment research [1] and theoretical studies of their properties are therefore necessary to enhance the ongoing effort for mucine-based medical applications.

Single mucin particles are made of repetitive domains, some of which are specialized in forming disulfide bridges. Owing to this facts a coarse-grained representation can be proposed. To better understand the dynamics of mucus net forming and its structural properties it is essential to study a multi-chain system with interactions between different domains evaluated accordingly.

A coarse grained off-latice model was introduced due to the size of the examined system. A Monte Carlo sampling algorithm based on the Metropolis was employed with a simulating method based on Backrub [2] move, commonly used for protein backbone rotations. Results including radius of gyration scaling and mean squared displacement behaviour were tested against universal scaling laws to ensure model corectness [3].

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Life-time of $^{\bullet}$OH radicals generated in water by ionizing radiation – comparison of experimental and simulation results with theoretical predictions

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The role of smart polymer materials with complex architectures in the market systematically increases. They have been found as attractive alternative for classical materials in many fields such as medicine, pharmacy, micro-, nano- and bio-engineering: electronics, opto-electronics, mechanics, fluidics and others. Radiation-induced synthesis of polymer materials offers many advantages such as: high-efficiency, purity and possibility of simultaneous sterilization. Playing with irradiation dose and dose rate, composition of reaction mixture and reaction conditions one may control product properties such as molecular weight, structure or cross-link density [1].

Radiolysis of water is a process resulting in generation of hydroxyl radicals $^{\bullet}$OH and hydrogen atoms. These two chemically active species may initiate many secondary processes including polymerization, cross-linking, degradation and others [2]. In a case of radiation-induced synthesis of polymers conducted in aqueous environment, especially at a high dose rate (as is the typical condition for industrial electron-beam irradiation), an important factor is the reactivity of hydroxyl radicals with the substrates in relation to self-recombination of $^{\bullet}$OH [3]. Kinetics of these reactions is also important in studying radical polymerization and cross-linking by pulse

methods, such as PLP-SEC and PEP-SEC where polymerization process is initiated by a sequence of short pulses of energy [4,5].

This work is a first step of a project on developing simulation tools based on the Dynamic Lattice Liquid (DLL) model [6,7] for analyzing polymer systems undergoing cross-linking processes and finally forming continuous or discontinuous three-dimensional polymer networks. The results of Monte Carlo simulations based on DLL model will be compared with kinetic simulations (CKS) [8] and experimental results. All obtained data will be discussed in light of theoretical predictions assuming classical second-order kinetics of $^{\bullet}$OH radicals recombination.

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Automatic Code Generation for Quantum Chemistry Calculations on Graphical Processing Units

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The complexity of computational kernels in quantum-chemical calculation calls for methods of describing the formulas and algorithms in a high-level, easy to understand and maintain way instead of relatively low-level description possible in typical, general-purpose programming languages. The issue is even more emphasized by the advent of general-purpose computing on graphics processing units (GPGPU); to take advantage of performance offered by the architecture, reimplementation of the computational kernels is necessary. While there are some attempts to use automatic code generation in the computational chemistry software, the technique is not very often used in typical quantum-chemical programs. The distinct exception is made by the applications to the tensor contractions required in the practical formulations of many-body theories (Configuration Interaction, Many-Body Perturbational Theory and Coupled Clusters methods), where this approach became quite popular[1].

The required level of abstraction is provided by Computer Algebra Systems (CAS), which are programs for symbolic manipulation of

mathematical expressions. A representative member of the CAS family is Yacas[2]. While not as widespread as other, more established CAS engines, the system has been already used in the context of computational chemistry[3]. We selected it mainly because of its availability, portability, and simplicity. In particular, it has a built-in code generator for the C language, and adding such functionality for other languages of interest was straightforward.

We present a Yacas-based application of code generation techniques, including general as well as GPGPU-specific optimizations, for some of the most challenging implementation tasks present in typical quantum-chemical software, namely the calculations of electron-repulsion integrals (ERI) and their gradients as well as exchange-correlation functionals. Additionally, we discuss the reorganization of the Fock matrix construction to ensure optimal execution on GPGPU architecture and provide preliminary benchmark results[4].

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ARUZ Dedicated Firmware

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The efficiency of the ARUZ performance is achieved by low-level optimization of its resource usage. While the configuration of the FPGAs working as control modules is fixed, each simulation variant has its own set of bitstreams for the FPGAs working as computational modules. Such an approach is justified since the configuration of all computational modules takes only several minutes, while the time required for simulation is counted in dozens of hours. From this point of view it is worth applying any optimization of computational module configuration in order to achieve maximum possible efficiency.

To conclude, the ARUZ efficiency is based on its specific components, which makes it a high-performance dedicated machine On the other hand, such an approach, based on custom elements, requires a particular methodology of debugging, especially if the scale of the machine is taken into consideration.

The poster demonstrates techniques applied to achieve the optimised HDL description for each simulation variant and to verify its behaviour.

Geminate electron-hole recombination in discrete molecular systems. A semi-empirical theory based on simulation results

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The classical theories of geminate charge recombination – the Onsager theory [1] and its extensions [2,3] – are based on the continuous diffusion model and are therefore of limited applicability to discrete molecular media. A lattice theory of geminate electron-hole recombination is also available [4], but it does not provide convenient expressions of the recombination probability, and has not been found useful in analyzing experimental data. Moreover, the above theories do not take into account various important factors, such as the possibility of different charge transport mechanisms, the presence of a donor-acceptor heterojunction in photovoltaic systems, or the structure of this heterojunction. In such a situation, we think it is desirable to construct a convenient yet reliable empirical theory of geminate charge recombination that could describe this process, in terms of measurable parameters, in a wide class of systems. We attempt to build such a theory by combining computer simulation results with the predictions of the analytical recombination theories.

In the first stage of our work, we analyzed the geminate recombination process using various lattice models of the medium. We have found that the electron-hole escape probability can be conveniently expressed by an equation obtained from the extended Onsager theory with an added empirical factor. In the case of homogeneous systems, this factor is independent of the dielectric constant, lattice constant, and charge

mobility. However, it depends on the lattice coordination number and, to some extent, on the assumed form of the charge transport mechanism. In donor-acceptor heterojunction systems, the introduced empirical factor shows a power-law dependence on the product εd, where ε is the dielectric constant and d is the lattice constant. We have also studied the effect of heterojunction roughness on the electron-hole escape probability, and have found that this effect is not very strong.

In the next stage, we extended our considerations to amorphous systems. We modelled the geminate recombination process by simulating a hopping motion of an electron and a hole on amorphous atomic structures. The latter were obtained from separate Monte Carlo simulations that used model interatomic potentials (e.g. the Lennard-Jones potential). We have determined the electron-hole escape probabilities for such structures and have used these results to generalize our empirical theory to amorphous media.

This work was supported by the National Science Centre of Poland (Grant No. DEC-2013/09/B/ST4/02956).

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