ARUZ

Analyzer of Real Complex Systems

General description

ARUZ is a parallel computing machine, in which the role of executing elements - instead of traditional CPUs (Central Processing Units), as it is in commonly known supercomputers - play FPGA (Field-Programmable Gate Array) devices [5]. Due to high flexibility of FPGAs, ARUZ can be used for wide range of applications. Currently, ARUZ executes DLL (Dynamic Lattice Liquid) algorithm, which can be used for simulations of complex physio-chemical processes such as diffusion or polymerization [6].
ARUZ has a cylindrical shape and is composed of 20 panels [2], containing 12 rows of PCBs (Printed Circuit Boards) each, 12 of them in each row. In summary, there are 144 PCBs in each panel and 2880 PCBs in the entire machine (Figure 1). These PCBs are called DBoards (it is an abbreviation from Daughter Boards) and they are controlled by 1 MBoard (Mother Board). Each DBoard is equipped with 9 FPGAs (Figure 1, Figure 2). 8 of them (DSlaves) are used for computations while the remaining one (DMaster) controls their operation.

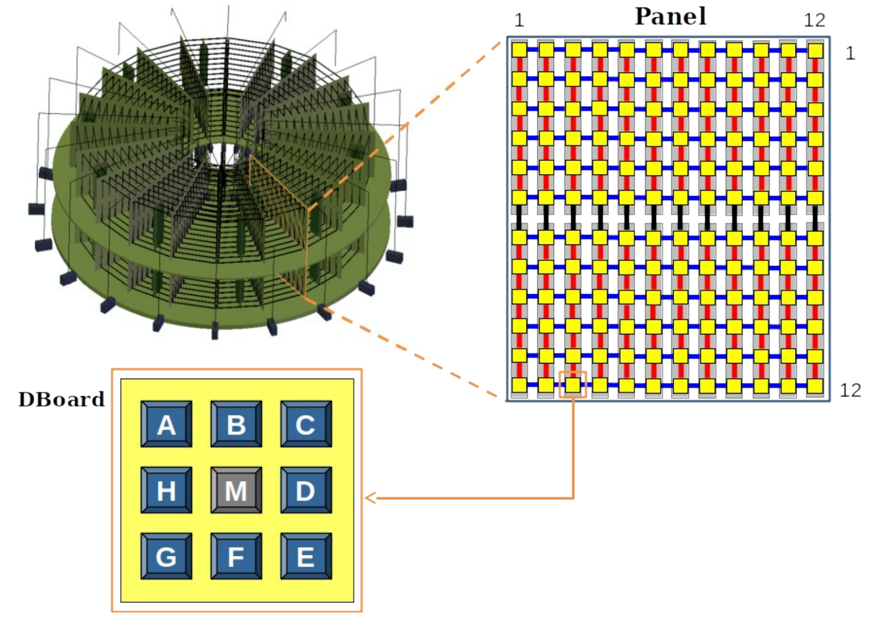

Figure 1. General ARUZ architecture

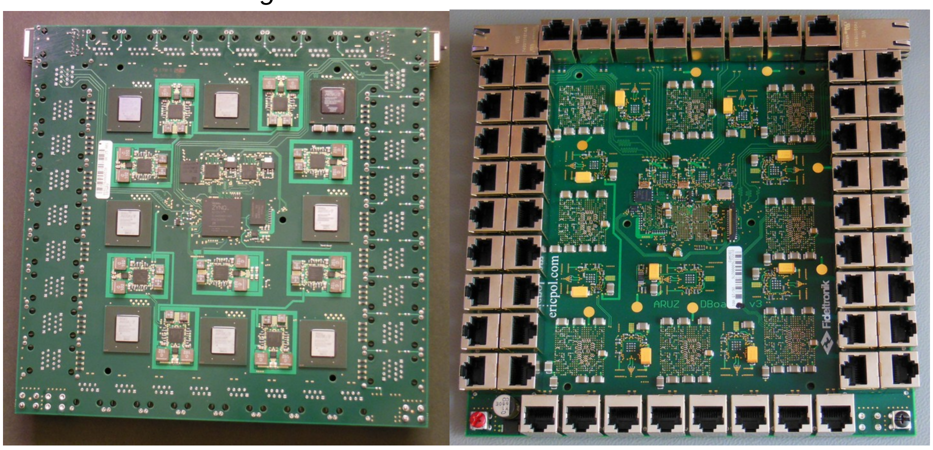

Figure 2. DBoard back (on the left) and front (on the right) side photo

In the contrary to DMaster, the configuration of which is fixed and loaded on startup, the configuration of DSlaves depends on the algorithm (or even the variant of the algorithm) to be executed. In case of DLL, in each DSlave the models of molecules or groups of molecules (e.g. atoms, particles, mers, etc.) are implemented. During the simulation these models exchange data and update their state. In that way they mimic – in the fully parallel manner – various interactions which can be observed in real fluids.

ARUZ innovations

The innovative character of ARUZ can be found in the following aspects:

- The way the ARUZ is constructed - this is an unique machine in which such a huge number of FPGAs (almost 26 000) exchange data in a parallel manner.
- The way the simulation space is mapped on executing elements (FPGA devices). Due to this innovative mapping [4] ARUZ is scalable even for periodic boundary conditions. Furthermore, such conditions can be obtained using arbitrary number of consecutive panels, treating the remaining ones as redundant (i.e. ready for use in case of failure of initially selected ones) [1].
- The way the FPGA devices are connected. In ARUZ one can distinguish 3 types of communication, each one matched to the system needs:
    - Global communication is dedicated for initialization of simulations and for acquisition of simulation results. Due to negligible influence of this communication on speed of computations, it is based on standard TCP/IP protocol and daisy-chained interconnections among neighboring boards in the row (Figure 3). In this way a comfortable user interface is achieved while the number of cables is relatively low.
    - Control communication is used for periodic synchronization of computations being executed by DBoards. This synchronization is performed by MBoard. The influence of control communication on the speed of computations is still low but slightly higher than in the case of global communication. Therefore, despite the fact that control communication is also based on daisy-chained interconnections (Figure 3) among neighboring boards in the row (giving the low number of cables needed for that purpose), the protocol of this communication is not the standard one. It is dedicated and optimized for specific character of transmitted data . In that way a low latency (signal propagation delay) of the synchronization is achieved.
    - Local communication is dedicated for the exchange of data among neighboring DBoards and it is crucial as far as the speed of computations is concerned. Therefore, except the dedicated protocol, this communication is based on direct interconnections of each DBoard with 6 DBoards in the nearest neighborhood (Figure 4) [3]. This gives admittedly almost 70 000 of cables (Figure 5), but results in high efficiency of data exchange.
- The way the algorithm is implemented. The configuration of DSlaves reflects the needs of the algorithm being executed. This gives the following profits (in comparison to the approach based on universal CPUs):
    - higher speed of computations
    - lower resource usage per one modeled system unit (model of molecule, etc.), so more units can be implemented
    - lower energy consumption

These effects are quite common for systems based on FPGA devices but they were never used on that scale before.

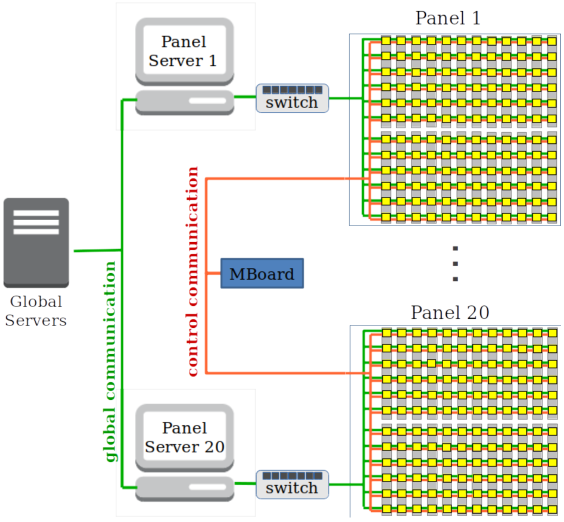

Figure 3. Global and control communication

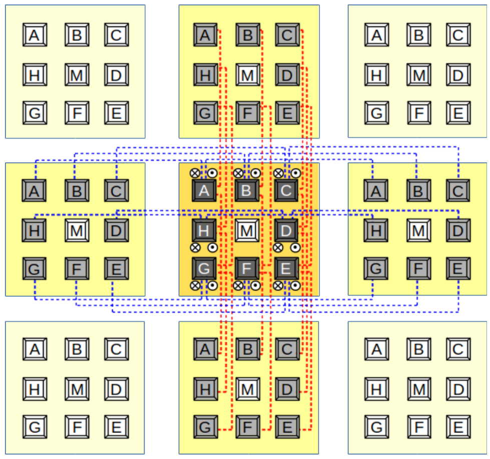

Figure 4. Inter-board local communication: interconnections among DBoards placed on the same panel are marked using dashed lines, inter-panel connections are marked with ⊗⊙ symbols.

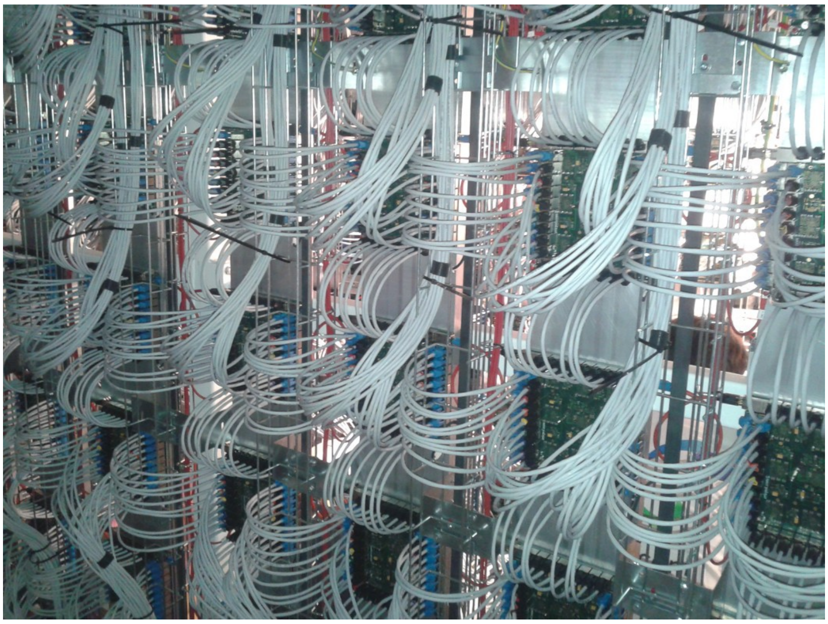
Figure 5. Photo of inter-board local communication cables

Application area

With the currently available configuration implementing the DLL algorithm, ARUZ can be used in simulations of complex physico-chemical processes occurring in liquid systems, such as: modelling of synthesis processes leading to complex macromolecular systems, chemical reactions in complex environments, dynamics of simple and complex liquids (like polymer systems), surface and interfacial effects, thin layers, macromolecules in confined space, adsorption at surfaces, effects of various macromolecular architectures on self-organization, molecular and macromolecular aggregation, clustering, heterogeneous media, microphase separation, nanoscale effects in all kinds of soft matter, behavior of multicomponent systems, composites and mixtures.

It is worth noting that due to the size of ARUZ, the performed simulations are characterized by high fidelity of reflecting the real phenomena. Therefore they can be used not only for proposing scientific hypotheses but also for industrial research.

Considering wide capabilities of ARUZ resulting from the configurability (flexibility) of its executive elements (FPGAs) it must be stressed that - apart from the currently implemented DLL algorithm - there is a wide range of computational problems (e.g. big data analysis, cryptography, artificial intelligence, etc.), for which ARUZ seems to constitute an attractive alternative to existing supercomputing systems.

Taking into account the specific topology of ARUZ interconnections, it seems to be the most predestined for solving problems with high locality of calculations (with data exchange only in the nearest neighborhood of computing elements) and problems that can be executed in parallel. A wide range of algorithms meets this criterion. One example is LBM (Lattice Boltzmann Method) for analyzing fluid mechanics. Initial tests have proved high efficiency of ARUZ executing this algorithm [7]. Among other algorithms, engineering lattice methods and all kinds of Monte Carlo algorithms can be mentioned, where mutual interactions of constituent elements of simulated system take place in parallel.

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