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Modelling with cellular automata: problem solving environments and multidimensional applications

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Chapter 5. Summary, Discussion and Conclusions

The work presented in this thesis addresses a special class of problem solving environments, which can be called cellular automata based modelling environments. Utilizing natural parallelism of cellular automata, such tools represent powerful facilities for modelling large scale complex phenomena in many application domains from science and engineering to economics and social sciences.

A lot of representatives of this class were created in last several decades. It may seem that authors of these facilities are not using the experience of each other, trying to reproduce marginally the same functionality in each of the cellular automata based modelling environments. Design of a universal, extensible and handy tool of this class requires a deep study of both fields: a problem solving environments common functionality and general expectations from the cellular automata modelling facility. Creation of significantly beneficial and conceptually new cellular automata based modelling environment CAME_{&L} is a central thread, which runs through this thesis.

In Chapter 2 we pose the following scientific question: what are the invariant requirements for a general cellular automata based modelling environment? To answer we united known requirements for the problem solving environments with the needs of researchers, who use cellular automata for computational models creation, and obtained a list of nine common requirements. After this we compared existing cellular automata based modelling environments versus this list to find out the flaws in their functionality and feature sets. The fact that all nine requirements were taken into account by some of existing tools allows to conclude that we formed a list of the invariant requirements for a general cellular automata based modelling environment. But none of the existing facilities totally satisfy all of them*.

The main bottleneck we point out is the niche specialism of each distinct existing environment. Most of them have latent orientation on a specific domain, or have significant restrictions allowing a distinct subclass of the cellular automata. At least, usually tools support grids of limited dimensionality, have predefined sets of neighbourhoods, possible cells' states etc.

We have motivated the necessity of a new environment called "CAME_{&L}" (the "Cellular Automata Modelling Environment & Library"), which represent a next level

*One may say that in Table 2.1 JCASim and SIMP/STEP (alongside with CAME_{&L}) got positive marks for all the requirements, but, as it is written above that table, the tool gets positive mark even if there was any step made in the direction of the requirement. This does not mean that the tool satisfies it totally.

problem solving environment in this field. CAME_&L allows to model even a wider class of systems than “cellular automata”. It was achieved with the help of the cellular automata based computational experiment decomposition, which distributes the functionality of a general computational model between five independent components.

The fact that these components are independent plays a key role, allowing to assemble the automaton required for computational model from building blocks. If needed, one of the blocks can be modified or replaced.

We hope that creation of such a universal facility, which can be extended, incorporating new algorithms, approaches and technologies, can stop the process of endless and wasteful creation of new cellular automata based modelling environments, giving the community a common tool. This would streamline solutions interchange and knowledge sharing.

To prove that CAME_&L is suitable for this, we present examples of its usage to produce scientific results, solving both theoretical and practical problems in one-, two- and three-dimensions.

Chapter 3 is devoted to its applications for the theoretical research and consists of two major sections. In Sect. 3.1 the classification of structures generated by one-dimensional binary cellular automata from a single seed have been performed. We juxtapose all 256 possible structures of this kind and group them, basing on different invariant operations. In this case CAME_&L allows to answer following scientific questions: how many and what kind of classes of equivalence can be distinguished among these structures? What is the number of really different shapes of structures, which do not represent mirror reflection, inversion or offsets of each other? Seventy variants of classifications have been performed and numbers of classes were calculated for each of them. According to the research we made a conclusion that there are 54 different kinds of shapes of structures generated by one-dimensional binary cellular automata from a single seed. In addition, it was shown that it is possible for a structure generated by an automaton with cells, which have memory, to belong to the same class as a structure, generated by an automaton with memoryless cells.

Another theoretical application is presented in Sect. 3.2. Cellular automata based computational experiment decomposition, which lies in the basis of CAME_&L design, offers to detach metrics into a separate part of the computational model definition. This gives an opportunity to use non-standard coordinate systems seamlessly. We offer to call a mapping of multidimensional grid structures into one-dimensional as “generalized coordinates” introduction.

CAME_&L allows to test and study different methods of generalized coordinates introduction, providing a universal way of data storage for the completely different grids. The only thing need to be changed for the particular grid is a set of expressions for the neighbours calculation. These expressions are the main content of a metrics component.

We have considered cellular automata with two-dimensional grids, composed of regular polygons. There are three possible grids of this kind: grid of triangles, squares, and hexagons. For each of this grids we proposed so called “spiral generalized coordinates”, which represent helical enumeration of cells around the one, which was chosen as an origin of coordinates. For each of grids there is a formalism, which gives ex-

PLICIT expressions for main neighbours lookup, when other neighbours can be found recursively. We demonstrate that such enumeration is mostly effective for the grid of hexagons, because all cell's neighbours are main on it. At the same time, it shows the worst productivity for the grid of triangles, because for this case only one quarter (3 of 12) of neighbours are main. That is why we propose a special way of the generalized coordinates introduction for the grid of triangles.

Six triangles can compose a hexagon. Consequently we can consider a metagrid of hexagons over the grid of triangles. Effective spiral generalized coordinated for the grid of hexagons can be introduced on the metagrid. Final generalized coordinate of a triangle is obtained as a composition of its index inside the hexagon and a coordinate of containing hexagon on the metagrid. Such approach outperforms even spiral generalized coordinates for the grid of squares.

Usage of generalized coordinates give an opportunity to enlarge the grid easily, because appending of cells to the end of a chain is much simpler than the reallocation of a multidimensional block structures. Moreover, in this case the state always presents a serial data and can be serialized straightforwardly.

At the same time, cellular automata are general models of parallel computations with in principle infinite extent of parallelism. The same functionality could be achieved with the help of infinite amount of Turing machines [23, 24]. Using the generalized coordinates a system with infinite extent of parallelism can be mapped to a system of finite quantity of Turing machines. A single machine used to represent a data storage (a tape) and finite quantity of machines are used for neighbours calculation and synchronization. Exact amount of machines depends on the implementation.

Generalized coordinates introduction along the space-filling curves [93] were widely used in computational physics for the numerical methods. Such enumeration optimises the calculations for the processor's stack [94]. Being executed on the modern hardware, the overheads of the offered generalized coordinates introduction methods are neglectable.

Chapter 4 demonstrates an application of CAME_&L for a practical task: three-dimensional tumour growth modelling. A complex multiscale process of tumour growth can be divided into a number of interconnected subphenomena. Deep overview of these subphenomena and existing models brings us to a conclusion that tumour natural shrinkage, which requires special attention, is deliberately neglected by models. That is why we demonstrate its relevance and influence on a growth regime. This rises a question about the validity of models, which neglect this phenomenon [†], because its influence is significant even from the resulting volume point of view.

Several approaches to the tumour shrinkage modelling are presented and comparatively studied. Some innovations, which can look as nonsense from the biological point of view were introduced for computational reasons. Their influence to the realism of the model was the third scientific question, which had been posed in Sect. 1.4: does purely computational tricks influence the realism of in silico tumour growth? CAME_&L gave an opportunity to conclude that this influence is negligible on the early stages of avascular tumour growth. We demonstrated that the substitution of

[†]Among the models, which were subjected to a review, only the one made by Dorman et al. [99, 107] accounts it on the cellular mesoscopic level.

the chain-pushing by looking for a vacant place using random walking does not influence the growth regime. This substitution results essentially in the abnormality of cells distribution from the biological phases point of view. Majority of outermost cells will be in G1 phase, when in real system there is no such extremum of G1-cells concentration on tumour surface. But the point is that exactly for the outermost cells this does not matter, because they would not be subjected to quiescence or necrosis in closest time, because they are close to the nutrition source.

In addition we presented a tumour successful mitoses rate study. Having no ability to measure such microscopic parameter in real biological system, we can draw some conclusions about its magnitude, basing on the simulation performed with CAME_&L and in vitro experiments of larger scale [164]. Our results suggest that at least 55% of inner proliferating tumour LoVo cells are dividing.

In Sect. 4.4.2 we use a value of the successful mitoses rate, which was computed during the simulations as a rate of the successful random walks from an inner malignant cell outside. A length of the walking trajectory was limited by a squared distance from the cell to the geometrical center of the tumour. The artificially computed result was 70% and it falls into the range of possible rates.

Among the overviewed models we have described another look to tumour growth modelling, which we have used [109, 110]. This approach is based on the cancer stem cells conception. Our work demonstrates that hierarchical organization of malignancies significantly contributes to the invasive morphology and increased heterogeneity of tumours. Accounting stem cells is a crucial issue for better understanding tumour biology and to improve current cancer treatments.

Presenting CAME_&L applications for the theoretical and practical research, we have also demonstrated its usability for one-dimensional (Sect. 3.1), two-dimensional (Sect. 3.2), and three-dimensional (Chapter 4) problems. This proves the fact that CAME_&L is a universal and powerful problem solving environment suitable for a complex research in a wide spectrum of scientific areas.

In future research we plan to continue applying CAME_&L to the tumour growth modelling, studying the later stages of neoplasms formation. At the same time different approaches to the generalized coordinates introduction should be tested and compared. Moreover, we are planning to present research in new fields of cellular automata application, done with CAME_&L.