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Evolutionary Computing Project

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Final Report for the Evolutionary Computing Project (LDRD-CD 97621)

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Abstract

This report summarizes LDRD-funded mathematical research related to computer simulation, inspired in part by combinatorial analysis of sequence to structure relationships of bio-molecules. Computer simulations calculate the interactions among many individual, local entities, thereby generating global dynamics. The objective of this project was to establish a mathematical basis for a comprehensive theory of computer simulations. This mathematical theory is intended to rigorously underwrite very large complex simulations, including simulation of bio- and socio-technical systems. We believe excellent progress has been made. Abstraction of three main ingredients of simulation forms the mathematical setting, called Sequential Dynamical Systems (SDS): 1.) functions realized as data-local procedures represent entity state transformations, 2.) a graph that expresses locality of the functions and which represents the dependencies among entities, and 3.) an ordering, or "schedule" according to which the entities are evaluated, e.g., "updated". The research spans algebraic foundations, formal dynamical systems, computer simulation, and theoretical computer science. The theoretical approach is also deeply related to theoretical issues in parallel compilation. Numerous publications were produced, follow-on projects have been identified and are being developed programmatically, and a new area in computational algebra, SDS, was produced.

Background and Research Objectives

Decision, management and design problems drive the need to simulate large systems such as the national electrical-, communications-, and transportation infrastructure as well as conventional warfighting scenarios, or strategically balanced nuclear force configurations. Moreover, large physical systems, biomolecular and biosystems analysis as well as topics in neuroscience, evolutionary- and population biology are increasingly investigated with simulation. Thus the use of simulation in science or system analysis involves the support of both discovery and decision-making activities. Simulation-based scientific/analysis work in socio-technical systems (those possessing physical, technological, and human components) is often characterized by a lack of detailed theoretical knowledge of the systems being studied, especially in comparison to the principles and concepts that serve to guide modeling and computation in purely physical sciences. In this situation, it is crucial that the representational tools themselves are well understood and theoretically grounded. However, rigorous foundations for simulation will importantly affect even simulation-based research in the physical sciences. For example, distributed implementations of a simulation of a physical system sometimes can be interpreted as a *simulation* of a conventional algorithm.

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Against this backdrop, we have developed a theoretical framework for computer simulations based on a new class of dynamical systems: sequential dynamical systems (SDS). SDS are maps obtained by composing a collection of local functions in a specific order, where local means that only the state-values of neighbors defined by a fixed base graph are relevant. Accordingly, the base graph, the structure of the local functions and their ordering are the basic elements of an SDS. The basic objective of our investigation is to understand how dynamical properties of the simulation depend on underlying rules, their structural and logical constraints and, in particular, the ordering in which these rules are iterated. We succeeded in relating symmetry properties of the underlying dependency graph to symmetry properties of a corresponding simulation over that graph. The analysis breaks into two basic approaches, one a purely combinatorial study of the dependency structure without specific reference to the particular local maps; the other focuses on phase space properties of particular local maps in certain classes of dependency graphs.

We found, in the course of our investigation, that the structure of a certain genotype-phenotype mapping is of central importance for the search for the "right" order in which a simulation has to be updated. This genotype-phenotype map turned out to be closely related to a map arising in the context of folding molecular sequences into their corresponding spatial structures. This establishes an interesting link between mathematical biology and our framework and has led to a series of studies on random subgraphs of n -cubes, random subgraphs of Cayley graphs, acyclic orientations of random graphs and neutrality in fitness landscapes.

Additionally, SDS have decomposition properties that are mathematically very closely related to Cartier-Foata's

Normal Form arising in the context of partially commutative monoids in connection with parallel compilation of computer programs.

Scientific Approach and Accomplishments

Some selected examples of results and accomplishments are:

1. SDS results pertaining to representation, validation and parallelization of a simulated system:
 - an upper bound on the number of "dynamically different" simulations generated from a fixed object library.

- general phase space properties of SDS over arbitrary graphs induced by certain local Boolean functions.
- characterization of invertible SDS and
- analysis of fixed points of SDS.

2. Other results relating to evolutionary molecular biology:

- the structure of a certain genotype-phenotype mapping is of central importance for the search for the "right" order in which a simulation has to be updated.
- this established an interesting link between mathematical biology and our framework and has led to a series of studies on random subgraphs of n-cubes, random subgraphs of Cayley graphs, acyclic orientations of random graphs and neutrality in fitness landscape.

3. Moreover, we have begun to apply the SDS set-up to various very difficult engineering problems:

- detailed analysis of large packet-switched communication systems.
- analysis of interdependencies among critical national network infrastructures.

4. The mathematical content of SDS is entirely new in its own right and will form the basis for graduate coursework in the mathematics department at New Mexico State University beginning in the Fall term 1999.

5. University of Trondheim, Norway will grant the first Mathematics Ph.D. in SDS, in May 2000 to Henning Mortveit, who has studied and helped develop the topic with Reidys and Barrett as a GRA in TSA-SA.

Selected publications produced by the Evolutionary Computation Project

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9. Barrett C.L. and Mortveit H. and Reidys C.M., Elements of a theory of simulation {III}: sequential dynamical systems, Appl. Math. and Comp., 1999, in preparation
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12. Reidys, C.M. and Stadler, P.F., Neutrality in Fitness Landscapes, Appl. Math. Comp., 1999, in press
13. Reidys, C.M. and Stadler, P.F. and Schuster, P.K., Generic Properties of Combinatory Maps and Neutral Networks of {RNA} Secondary Structures, Bull. Math. Biol., 1997, vol 59, nr 2, p. 339 - 397.
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18. S. Kopp and C.M. Reidys and P.K. Schuster, Exploration of artificial landscapes based on random graphs, in Self-Organization of Complex Structures: From Individual to Collective Dynamics, Gordon and Breach, 1996, p. 179-187.

Follow-on Projects

Participating in Infrastructure Interdependency Project

Participating in Electrical Power Grid Analysis Project

Mobile Digital Communication System Analysis Project with Motorola

PI's

Chris Barrett, TSA-SA, Simulation

Christian Reidys, TSA-SA, Mathematics

Collaborators

G. C. Rota, MIT, Algebraic Combinatorics (deceased)

W. Chen, T-7 LANL/Univeristy of Nankai, Combinatorics

R. Laubenbacher, New Mexico State University, Algebra

Michael Waterman, USC, Mathematical Biology

P.K. Schuster, University of Vienna, Mathematical Biology

P.F. Stadler, University of Vienna, Mathematical Biology

Henning Mortveit, University of Trondheim, Algebra & Dynamical Systems

S.S. Ravi, SUNY Albany, Theory of Algorithms

Madhav Marathe, CIC-3, Theory of Algorithms & Simulation

Stephan Kopp, TSA-SA, Mathematical Biology