Second Year Dissertation Summary

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Abstract

This document summarizes the results produced in the course of the doctorate studies of the author in the period of November, 2013 to October, 2014. It is intended to use as a reference for the presentation on next October 28th, 2014 and not as a technical, detailed report of the results.

1 Introduction

Almost one year of research work involves a lot of (usually, failed) experiments and the reach of (few) results; still, the undertaken track of investigation usually reveals deeper and more important insights than the produced results.

For this reason, the present document describes, chronologically, the ideas and strategies tried by the author in order to prove the central thesis of his doctorate work (Section 2). It is certainly a *summary of investigative science* instead of a *report of results*.

2 Research Thesis

The *research thesis* is the premise the current doctorate research seeks to prove (or disprove) as its final product; in this context, it is never referenced as the text presented to the completion of the studies.

Hence, the research thesis of the current work can be stated, in the state of last year presentation, as

> demonstration of a mathematical equivalence between dynamics described by Metabolic P systems and electronics circuits, particularly digital ones.

So, the main goal was, under the author's perspective,

1. to produce a theoretical (*i.e.*, mathematical) result
2. in a form of a binary relation [7, 19, § 1.2 and 1.3; p. 9] that could compare
3. two or more classes (MP systems and digital electrical circuits, with possibility to expand to analog ones) of (dynamical) objects (or models) and
4. it was expected to be an equivalence relation [7, 19, p: 16; p. 9],
5. so models of one class could be converted to the other one.

This *mathematically driven research thesis* has guided the research work from its origin and is the key concept to understand the trajectory carried out.

Nonetheless, as a result of its own fate, the aforementioned research thesis has evolved and comprises not only its original statement, but also new ones—a discourse reserved for the Section 6.

3 Analysis of Analog Circuits

Since it was know by the author that analog circuits are computationally more powerful than digital circuits [18], the chosen approach consisted in finding a relationship between these types of circuits and MP systems.

Following the successful methodology of the group on previous projects[10, 11, 12, 13] and the extensive spectrum of signals processed by analog circuits, start a study the viability of constructing MP grammars that reproduces the behaviour of particular simple circuits; the strategy used for the MP grammar construction was to perform regression over the input and output signals time series of the circuits using the *Log Gain Stoichiometric Stepwise* regression algorithm [10].

Although four initial configurations of analog circuits were chosen for the tests, the RC with controlled input signal depicted in Figure 1 was the unique one used for them: its simplicity in design—the simplest

Figure 1: RC analog circuit with controlled input signal, as modelled in MATLAB Simulink.

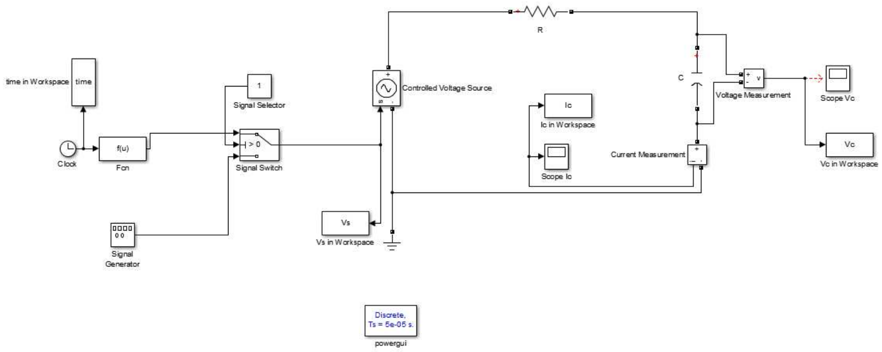


Table 1: Dictionaries used in the tests with the RC analog circuit with controlled input signal.

Name of the Dictionary	**Composition Rule**
All Functions	$D = F$
Trigonometric	$D = \{1, x, \sin(x), \cos(x)\}$
Complex Functions	$D = \{1, x, \exp(x), \frac{1}{1+\exp(-x)}, \lfloor x \rfloor\}$
Polynomial Functions	$D = \{1, x^n\}$ and redefined $n \in \{1, 2, 3, 4, 5\}$
Polynomial and Trigonometric Functions	$D = \{1, x^n, \sin(x), \cos(x)\}$
Composition of All Functions	$D = F \cup C$
Composition of Complex Functions	$D = F \cup C$ and redefined $F = \{1, x, \exp(x), \frac{1}{1+\exp(-x)}, \lfloor x \rfloor\}$
Composition of Trigonometric Functions	$D = F \cup C$ and redefined $F = \{1, x, \sin(x), \cos(x)\}$
Complete (All Possible Combinations)	$D = F \cup C \cup I$

analog circuit beyond the resistive ones—and in system's equation was crucial for its selection and enough to satisfy the investigation.

The tests consisted of three basic input signals (sine, square and saw-tooth ones) and regressions on three phases of the output signals (transient, steady state and whole signal) based on nine different dictionaries (see Table 1) containing enough properties to infer or approximate the curves; the dictionaries were constructed combining the three different structural sets, namely: the set of function $F = \{1, x^n, \sin(x), \cos(x), \exp(x), \frac{1}{1+\exp(-x)}, \lfloor x \rfloor\}$, the set of composite functions $C = \{f \circ g : f, g \subseteq F\}$ and the set of inverse functions $I = \{\frac{1}{h} : h \in F \cup C \setminus x\}$, with $x \in \{V_s, V_c, I_c\}$ and $n \in \{1, 2, 3\}$.

As the general result, MP regression has failed to infer the correlation between the input and the output signals with the given (and not trivial) dictionaries, except for rare situations. In particular, the transient phase of the output signal, side effect of the differential equation that models the analog circuit, is never inferred. (Also, steady state of square and saw-tooth signals are also not properly inferred.)

Disappointed with the results, alternative strategies were used, including: (i) non-linear optimization (using CMA-ES algorithm [5]); (ii) attempts of new dictionaries, such as the Kolmogorov-Gabor polynomials and Maclaurin series; (iii) analysis under the *Fourier transform* perspective. While the first to ideas has failed the tests, the *"Fourier idea"*—which can be seen as a MP version of the *fast Fourier transformer (FFT)*—got a special research development track.

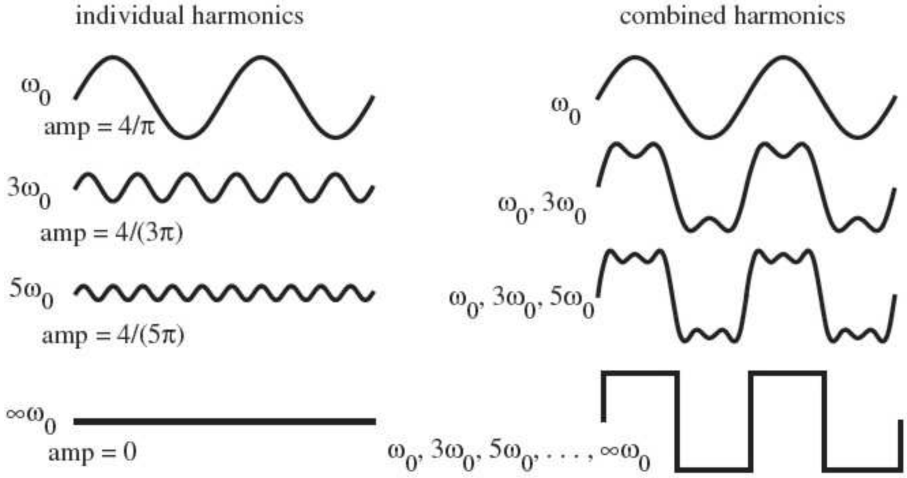
4 MP version of FFT

The Fourier transform is an invertible operation that changes the domain space of a given signal from the time to the frequency one. It is deeply connect to Fourier series and harmonic analysis.

In circuit analysis, Fourier transform (actually, the *Laplace transform*, a more general but similar integral transform) is used to transform integro-differential equations in the time domain to algebraic equations in the frequency domain, simplifying its solution in this new domain and, through the invertibility property, return to the time domain with the proper solution of the equations.

The application of Fourier analysis to circuit and signals studies, which involves harmonic compositions as depicted in Figure 2, has inspired the replication of the *fast Fourier transform* (FFT) algorithm in a

Figure 2: Harmonic composition of the square wave. [2]



metabolic P context. In this perspective, the central idea is to reproduce the relation input and output signals in the frequency domain, inferring the harmonic frequencies (*i.e.*, sines and cosines of different frequencies) that compose the signals, as well as their input-output rules [8, p. 155].

After some studies in both MP systems (particularly Goniometricus dynamics) and discrete Fourier transform (including diverse algorithms for FFT), a MP version of the fast Fourier transform were successfully produced which even outperforms the state of the algorithm, FFTW [3], in the accuracy tests (see Table 2).

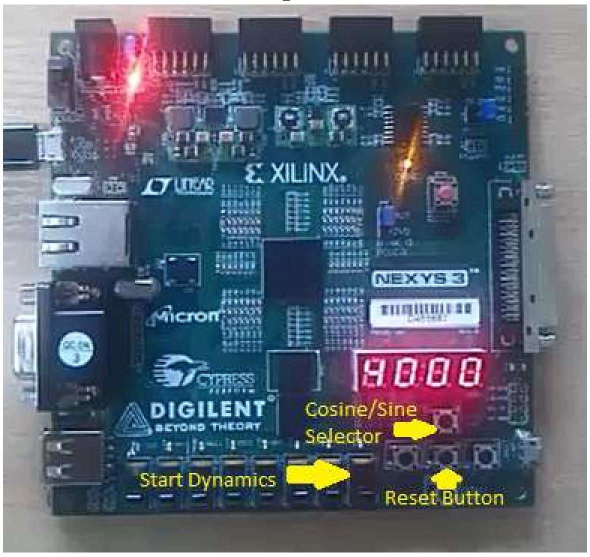
For the speed benchmark, some efforts were putted in to converting the existing code to native one so it could produce a fair comparison with FFTW algorithm (implemented in C and used as a compiled library by numerical studios such as MATLAB [15, § More About]).

However, with the six-month period abroad in Lithuania, the project has been paused with ambitions to restart it later this year.

Table 2: The retrieved frequencies using the FFT and MP-FFT methods.

Signals	**Frequency**	**Numerical Frequency**	**FFT**	**MP-FFT**	**MP-FFT (MATLAB)**
1	20	20	20	20	20
2	$20 + df$	20.5	20.5	20.5	20.5
3	$20 + \frac{3}{4} \cdot df$	20.375	20.5	{20, 20.5}	{20 20.5}
4	$\{20, 47\}$	$\{20, 47\}$	{20, 47.5}	{20, 47, 47.5}	{20 47}
5	$\{20 + df, 47 + 3 \cdot df\}$	$\{20.5, 48.5\}$	{20.5, 49}	{20.5, 48.5, 49}	{20.5 48.5}
6	$\{20 + \frac{3}{4} \cdot df, 47 + \frac{2}{3} \cdot df\}$	$\{20.375, 47.\overline{3}\}$	{20.5, 47.5}	{20.5, 47.5}	{20.5 47.5}
7	20 + noise	20 + noise	{2, 3, 5, 7, 8.5, 10, 12, 14, 15, 16.5, 17.5, 18.5, 20, 22.5, 23.5, 24.5, 25.5, 26.5, 27.5, 29, 30.5, 32.5, 34, 35, 36.5, 38, 39.5, 41.5, 44, 45, 47, 48}	20	20
8	$20 + df$ + noise	20.5 + noise	{1, 3.5, 4.5, 6, 7.5, 10, 12, 14, 15.5, 17.5, 19, 20.5, 21.5, 23, 24, 25.5, 27, 28, 30, 32, 33, 34.5, 36, 37.5, 40, 42, 43, 44, 47, 48, 49.5}	20.5	20.5
9	$20 + \frac{3}{4} \cdot df$ + noise	20.375 + noise	{1.5, 2.5, 5.5, 6.5, 8, 9.5, 11, 12, 13, 15, 16, 17.5, 20.5, 22.5, 23.5, 25.5, 26.5, 27.5, 28.5, 29.5, 31, 32, 33.5, 34.5, 36, 37, 38, 40, 42, 43, 44.5, 46, 47, 49}	20.5	20.5

Figure 3: Digilent Nexus V3 board running the Goniometricus MP dynamics[§ 3.3.1][8].



5 (The Short, Long Road on) Digital Circuits

Along with the change of research group, a change of perspective on the academic research has also came. In the Vilniaus Gemidimo Technikos Universitetas (VGTU) in Vilnius, Lithuania, under the supervision of Prof. Darius Navakauskas, it was planned to study a correlation between MP systems and VHDL primitives in direction to find an equivalence between the system and digital circuits. The choice on digital circuits and VHDL design made by the hosting group relied on their extensive knowledge in both fields, lately focusing its application on neural networks embedded in FPGAs.

As presented in the past [4] (and also more recently [14]), there were positive suspicions of the feasibility of implementation of MP systems in digital hardware, but no attempt had been made to that moment. With no surprise, nonetheless, versions of important MP dynamics were designed in FPGA through VHDL hardware description (Figure 3). Unexpected, though, was the observation that MP notation eases the implementation of dynamics in VHDL and provides a structured framework for MP-to-schematics translation (Figure 4).

In possession of these new knowledge and working examples, the pursuit for a generalization of the results through a formal equivalence relation between the MP systems and digital systems has taken place with a series of attempts involving a wide range of mathematical and computational knowledge, such as *dynamical systems, automata theory, computability, logic synthesis, control theory, algebraic groups, commutative diagrams* and *category theory*, to name a few.

Although some lights were shed in the subject with the support of *(general definition of) dynamical systems, commutative diagrams* and *category theory* (see Figure 5), it was not possible to prove (in the period abroad) the formal equivalence relation between the systems because of issues like (i) too general domains on the input and output sets of MP systems; (ii) general-first approach of the proof; (iii) confusion on separating concepts of proof of equivalence relation and convergence of systems, among others.

The chase of a nonexistent formal proof for a given hypothesis is not as trivial as the above paragraphs summarize: it is an intensive (intellectual) activity that frequently ramifies in a series of attempts involving not-so-obviously correlated subjects; the aforementioned effort, for example, took three and a half months of the author with several communication exchange among, at least, eight other researchers.

A change of perspective, however, has practically solved the theoretical quest: derived from a past work of Manca and Lombardo [9] has arisen an equivalence between a particular subset of MP systems and register machines, defining it as a computationally universal device. By the other side, digital systems, codified in sequential logic, are also computationally universal, particularly through the equivalence with Universal Turing Machines [7, § 5.2]; hence, by the Church-Turing thesis [7, 19, § 5.1; p. 181], both systems are equivalent and the question of the proof may be considered as settle down.

In the next months, as a matter of illustration and continuity of the research, examples of general devices in both systems will be designed in order to compose a didactical step-by-step proof of the equivalence.

Figure 4: An arithmetical network of the Goniometricus MP dynamics.

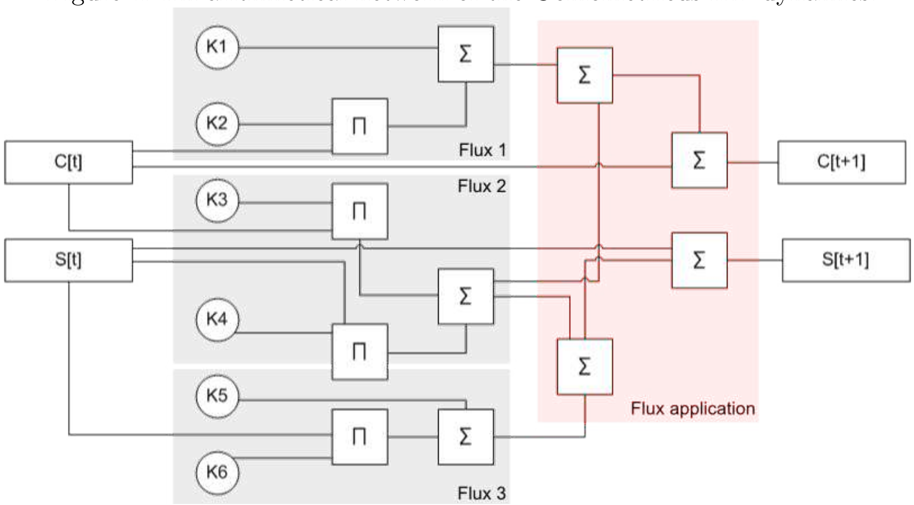


Figure 5: Commutative diagram of an attempt to prove the equivalence relation between MP systems and digital systems through dynamical systems representation [6, Definition 2.1.1].

$$\begin{tikzcd}
T_{\mathcal{M}} \arrow[d, "id"] & U_{\mathcal{M}} \arrow[r, "\Phi"] \arrow[d, "round"] & X_{\mathcal{M}} \arrow[r, "id"] \arrow[d, "?"] & Y_{\mathcal{M}} \arrow[d, "round"] \\
T_{\mathcal{D}} & U_{\mathcal{D}} \arrow[r, "\Phi_{\mathcal{D}}"] & X_{\mathcal{D}} \arrow[r, "id"] & Y_{\mathcal{D}}
\end{tikzcd}$$

6 Perspectives on the Research

Initially, the proposal for this research project was relatively open and wide, proposing a theoretical final product, in the form of an equivalence relation, that could show the possibility of implementing MP systems—and, consequently, models of biological metabolisms—as instances of analog or digital electrical circuits (and vice versa), paving the way for an exchange of concepts and theories between biological and electrical fields.

One year later, part of this result (concerning the digital systems) has already been reached, even with working, real-world examples; for the remaining one, strong scientific arguments [18] suggest its rejection. So, arises the (rhetorical) question: *what is going to be next?*

For the short-term future, it is expected to understand and propose a general method (an algorithm) for the conversion of MP systems into schematics diagram of digital circuits without the need of an intermediate layer (VHDL design), analogous to the one proposed for gene networks [12, 13, § 7.3].

Parallelly, optimization on the MP-FFT algorithm are planned in order to make it competitive to the FFTW one, followed by other activities correlated with the whole research project (*e.g.*, supporting software for register machines and MP systems).

Finally, the author feels compelled to emphasize his observations on the importance of this research topic, specially in the face of the growing field of synthetic biology: in this young research area, the boundaries between electrical engineering, computer science and biology are getting narrower at a such fast pace that well-known vanguard institutions has started to heavily investing on it [16, 17, 1]. Hence, the present work gets inserted in a privileged position inside a context of demanding inovation, with the opportunity to define itself as one of the reference techniques.

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