Experimental simulation of quantum graphs by microwave networks - Closed and open systems

Michał Lawniczak, Oleh Hul, Szymon Bauch, and Leszek Sirko

Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warszawa, Poland
(E-mail: sirko@ifpan.edu.pl)

Abstract. We show that chaotic quantum graphs of connected one-dimensional wires can be experimentally simulated by irregular microwave networks consisting of coaxial cables. The spectra of the microwave networks are measured for undirected and directed networks. The directed networks simulating quantum graphs with broken time reversal symmetry consist of microwave circulators apart from coaxial cables. In this way the properties of the graphs such as the nearest neighbor spacing distribution and the lengths of periodic orbits are obtained. Furthermore, we present the results of numerical studies of the parametric level correlation function $c(x)$ for Neumann and circular orthogonal ensemble (COE) graphs. We also demonstrate that microwave networks with absorption can be used to investigate properties of open quantum systems which recently have been extensively studied in the context of transparent electronics and new biosensors. We report the experimental studies of the distributions of Wigner’s reaction $K$ matrix for the networks with preserved time reversal symmetry. Moreover, the enhancement factor for the networks simulating open quantum graphs with preserved and broken time reversal symmetry is experimentally evaluated. We demonstrate that the experimental results are in good agreement with the random matrix theory predictions.

Keywords: Microwave networks, Quantum graphs, Random matrix theory.

1 Introduction

Quantum graphs of connected one-dimensional quantum wires were introduced more than seventy years ago by Pauling [1]. The same idea was used later by Kuhn [2] to describe organic molecules by free electron models. Quantum graphs can be considered as idealizations of physical networks in the limit where the widths of the wires are much smaller than their lengths, i.e. assuming that the propagating waves remain in a single transversal mode. Among the systems successfully modeled by quantum graphs one can find e.g., electromagnetic optical waveguides [3,4], mesoscopic systems [5,6], quantum wires [7,8] and excitation of fractons in fractal structures [9,10]. Recently it has been shown that quantum graphs are excellent paradigms of quantum chaos [11–23]. More realistic open systems - microwave networks with moderate and
strong absorption strength $\gamma = 2\pi \Gamma/\Delta$, where $\Gamma$ is the absorption width and $\Delta$ is the mean level spacing, have been experimentally investigated in [24–28]. The distribution of the reflection coefficient $P(R)$ and the distributions of the Wigner reaction matrix [29] (in the literature often called $K$ matrix [30]) for networks (graphs) with time reversal symmetry (TRS) (symmetry class of random matrix theory $\beta = 1$ [31]) in the presence of moderate ($\gamma \leq 7.1$) and strong absorption ($\gamma > 20$) have been respectively studied in [24,25] and [26,28]. The results of the experimental study of the two-port scattering matrix $\hat{S}$ elastic enhancement factor $W_{S,\beta}$ for microwave irregular networks simulating quantum graphs with preserved and broken time reversal symmetry in the presence of absorption was reported in [27,28]. Other interesting open objects - quantum graphs with leads - have been analyzed in details in [14,15].

The paper [21] showed that using a simple experimental setup consisting of microwave networks (throughout the text we also use the names: microwave graphs or circuits) one may successfully simulate quantum graphs. The circuits are constructed of coaxial cables connected by microwave joints. Furthermore, to mimic the effects of the time reversal symmetry breaking in quantum systems it is sufficient to add the microwave circulators [27] into the circuits.

The analogy between quantum graphs and microwave networks is based upon the equivalency of the Schrödinger equation describing the quantum system and the telegraph equation describing the ideal microwave circuit. This paper continues the use of microwave spectroscopy to verify wave effects predicted on the basis of quantum physics, which for two-dimensional systems, thin microwave cavity resonators, was pioneered by [32] and further developed by [24,33–43]. The first microwave experiment specifically devoted to study of quantum chaotic scattering was reported in [44]. Later on a similar experimental technique was applied in the observation of resonance trapping in an open microwave cavity [45]. In the case of two dimensions the Schrödinger equation for quantum billiards is equivalent to the Helmholtz equation for microwave cavities of corresponding shape. Three-dimensional chaotic billiards have been also studied experimentally in the microwave frequency domain [46–50] but for these systems there is no direct analogy between the vectorial Helmholtz equation and the Schrödinger equation.

2 The telegraph equation on a microwave network

A general microwave network consists of $N$ vertices connected by bonds e.g., coaxial cables. The coaxial cable consists of an inner conductor of radius $r_1$ surrounded by a concentric conductor of inner radius $r_2$. The space between the inner and the outer conductors is filled with a homogeneous material having the dielectric constant $\varepsilon$. For frequency $\nu$ below the onset of the next TE$_{11}$ mode [51], inside a coaxial cable can propagate only the fundamental TEM mode, in the literature often called a Lecher wave.

In order to find propagation of a Lecher wave inside the coaxial cable joining the $i$–th and the $j$–th vertex of the microwave graph one can begin with the continuity equation for the charge and the current on the considered cable (bond) [52].
where \( e_{ij}(x, t) \) and \( J_{ij}(x, t) \) are the charge and the current per unit length on the surface of the inner conductor of a coaxial cable.

For the potential difference one can write down

\[
U_{ij}(x, t) = V_{2ij}(x, t) - V_{1ij}(x, t) = \frac{e_{ij}(x, t)}{C},
\]

where \( V_{1ij}(x, t) \) and \( V_{2ij}(x, t) \) are the potentials of the inner and the outer conductors of a coaxial cable and \( C \) is the capacitance per unit length of a cable.

Taking the spatial derivative of (2) and assuming that the wave propagating along the cable is monochromatic \( e_{ij}(x, t) = e^{-i\omega t}e_{ij}(x) \) and \( U_{ij}(x, t) = e^{-i\omega t}U_{ij}(x) \) one can obtain [52]

\[
\frac{d}{dx}U_{ij}(x) = -ZJ_{ij}(x),
\]

where \( Z = R - \frac{i\omega L}{c} \). \( R \) and \( L \) denote the resistance and the inductance per unit length, respectively. The angular frequency \( \omega \) is equal to \( 2\pi\nu \) and \( c \) stands here for the speed of light in a vacuum.

Making use of the equations (1-3) and the definition of \( Z \) for an ideal lossless coaxial cable with the resistance \( R = 0 \), one can derive the telegraph equation on the microwave graph

\[
\frac{d^2}{dx^2}U_{ij}(x) + \frac{\omega^2}{c^2}U_{ij}(x) = 0,
\]

where \( \varepsilon = LC \) [53].

It can be easily recognized that assuming the correspondence: \( \Psi_{ij}(x) \Leftrightarrow U_{ij}(x) \) and \( k^2 \Leftrightarrow \frac{\omega^2}{c^2} \), equation (4) is formally equivalent to the one-dimensional Schrödinger equation (with \( \hbar = 2m = 1 \)) on the graph with the magnetic vector potential \( A_{ij} = 0 \) [12],

\[
\frac{d^2}{dx^2}\Psi_{ij}(x) + k^2\Psi_{ij}(x) = 0.
\]

3 Integrated nearest neighbor spacing distribution

The equivalence of irregular microwave networks and chaotic quantum graphs with time reversal symmetry was checked in the paper [21]. In the recent paper Lawniczak et al. [27] additionally demonstrated that in order to mimic the effects of the time reversal symmetry breaking in quantum graphs it is sufficient to add the microwave circulators into the circuits. Microwave networks with circulators are also called directed networks. The important measure of systems’ chaotic behavior the integrated nearest neighbor spacing (INNS) distribution \( I(s) \) was evaluated experimentally for tetrahedral microwave networks
(number of vertices $n = 4$), simulating quantum graphs with time reversal symmetry [21], and hexagon directed networks ($n = 6$) simulating graphs with broken TRS [27]. Figure 1 shows the experimental set-up for measurements of spectra of hexagon directed networks which was used for evaluation of the integrated nearest neighbor spacing distribution $I(s)$.

The distribution $I(s)$ is defined as follows

$$I(s) = \int_0^s ds' P(s'),$$

where $P(s')$ [54] is the nearest neighbor spacing distribution.

Figure 2 shows the INNS distribution obtained for tetrahedral microwave networks (number of vertices $n = 4$) simulating quantum graphs with time reversal symmetry. The solid line represents predictions of random matrix theory obtained for Gaussian Orthogonal Ensemble (GOE), applicable for systems with a time–reversal symmetry. The dashed line denotes results characteristic for Gaussian Unitary Ensemble (GUE), used if the time reversal symmetry is broken [54]. Experimental curve (open triangles) was obtained by averaging over the set of 10 microwave graphs obtained by varying the length of one bond, which provided us with the total of 2220 experimentally measured eigenfrequencies. Figure 2 demonstrates that the INNS distribution is in a very good agreement with the GOE prediction.

Figure 2 also shows the INNS distribution obtained for the directed networks. The experimental curve (full circles) obtained by averaging over the
Fig. 2. Integrated nearest neighbor spacing distributions \( I(s) \) obtained for tetrahedral networks (open triangles) and hexagon networks (full circles) simulating, respectively, graphs with preserved and broken time reversal symmetry, are compared with the theoretical predictions for GOE (solid line) and GUE (dashed line).

set of 20 directed microwave hexagon networks \((n = 6)\) was compared to the predictions of GOE and GUE systems. It is seen that the experimental INNS distribution is in good agreement with the GUE prediction.

4 Lengths of periodic orbits in the network

The measurement of the spectra of the networks enables to calculate the lengths of periodic orbits in the network \([21]\). They were computed from the Fourier transform

\[
F(l) = \int_0^{k_{\text{max}}} \tilde{\rho}(k)\omega(k)e^{-ikl}dk,
\]

where \(\tilde{\rho}\) is the oscillating part of the level density and \(\omega(k) = \sin^2(\pi \frac{k}{k_{\text{max}}})\) is a window function that suppresses the Gibbs overshoot phenomenon \([38,55]\). Here \(k_{\text{max}}\) is the maximal value of the wave number within the interval where the eigenvalues of the network were evaluated. In order to extract the oscillating part of the level density \(\tilde{\rho}\) from the density of states \(\rho(k) = \sum_j \delta(k - k_j)\) the mean density \(\bar{\rho}(k) = d\bar{N}(k)/dk\) was subtracted.

The absolute square of the Fourier transform of the fluctuating part of the density of resonances \(|F(l)|^2\) for the network of the “optical” length 223.6 cm is shown in Figure 3. The lengths of the bonds of this network fulfill the following relations: \(a < b < c < d < e < f\). Results obtained from the experimental spectrum (solid line) are compared to the results obtained
Fig. 3. Absolute square of the Fourier transform of the fluctuating part of the density of resonances of the graph of the “optical” length 223.6 cm. Results of the experiment (solid line) are compared with the numerical results (dotted line). The assignment of peaks of $|F(l)|^2$ to simple periodic orbits is shown along with the length of the orbits. The “optical” lengths of the bonds of the graph: $a = 21.0$ cm, $b = 26.3$ cm, $c = 34.0$ cm, $d = 39.6$ cm, $e = 46.8$ cm, $f = 55.9$ cm.

from numerical calculations (dotted line). The absolute square of the Fourier transform $|F(l)|^2$ shows pronounced peaks near the lengths of periodic orbits. Figure 3 shows good agreement between the experimental and the numerical results.

The above experimental and numerical results clearly show that chaotic quantum graphs can be experimentally simulated by irregular microwave networks consisting of coaxial cables.

5 The autocorrelation function $c(x)$ of the level velocities

Hul et al. [56] demonstrated that for fully connected Neumann graphs (graphs with Neumann boundary conditions at vertices) there are some spectral statistics, e.g., the second order level velocity autocorrelation functions $c(x)$ and $\tilde{c}(\omega, x)$ that for larger graphs ($n > 6$) show deviations from the predictions of RMT for GOE. This important property of large graphs has been further investigated numerically in the recent paper [23] where fully connected Neumann and COE quantum graphs of different size were considered. COE graphs are characterized by the circular orthogonal ensemble boundary conditions. Here, we would like to demonstrate that for larger COE graphs the autocorrelation functions of velocities $c(x)$, in contrast to large Neumann graphs, show very good overall agreement with the random matrix theory predictions.
The autocorrelation function $c(x)$ of the level velocities is defined as follows:

$$c(x) = \left\langle \frac{\partial \xi_i}{\partial \bar{x}} (\bar{x}) \frac{\partial \xi_i}{\partial \bar{x}} (\bar{x} + x) \right\rangle,$$  

where $\xi_i$ are the rescaled eigenenergies of the graph, $x$ is the rescaled external parameter $X$ [56]. The average $\langle \cdots \rangle$ is performed over the parameter $\bar{x}$ and over all the energy levels. The autocorrelation function $c(x)$ measures the correlation of the level velocities which belong to the same energy level. We chose the change of the bonds lengths of a graph to be the external parameter $X$. For the graphs with the even number of bonds the lengths of all the bonds were changed, while for the graphs with the odd number of bonds we changed the lengths of all the bonds except the arbitrary chosen one.

In Figure 4 we show our recent numerical results for the velocity autocorrelation function $c(x)$ for Neumann (full squares) and COE (open circles) graphs with $n = 20$ vertices compared to the results of RMT for GOE (solid line). It is clearly seen that for large COE graphs with $n = 20$ vertices the velocity autocorrelation function $c(x)$ is very close to the RMT predictions. Oppositely, for Neumann graphs due to the importance of localization effects in graphs [23] a significant departure from the GOE prediction is observable.

6 Microwave networks with absorption

A network with no absorption and no leads to the outside world is a closed system. However, in a real microwave network there exist absorption and/or leads
which create an open system. Absorption in an undirected microwave network (without microwave circulators) and directed networks can be efficiently varied by changing the length of the cables [21] or by adding microwave attenuators [25].

6.1 Distributions of the reflection coefficient $R$ and the Wigner’s reaction matrix $K$

In this paragraph we would like to present the results of experimental study of the distribution $P(R)$ of the reflection coefficient $R$ and the distributions of imaginary and real parts of Wigner’s reaction matrix $K$ [29,30] for microwave networks with absorption that correspond to quantum graphs with time reversal symmetry ($\beta = 1$ symmetry class of random matrix theory [31]).

The $K$ matrix and the scattering matrix $S$ are related by

$$S = \frac{1 - iK}{1 + iK}. \quad (9)$$

Additionally, the function $K = -iZ$ and the scattering matrix $S = (1-Z)/(1+Z)$ are directly connected with the impedance $Z$, which has been recently measured in a microwave cavity experiment [57,58].

In the case of systems coupled by a single-channel antenna the scattering matrix $S$ can be parameterized as

$$S = \sqrt{R}e^{i\theta}, \quad (10)$$

where $R$ is the reflection coefficient and $\theta$ is the phase.

The properties of statistical distributions of the scattering matrix $S$ with direct processes and imperfect coupling were considered in several important theoretical papers [59–62]. The distribution of the $S$ matrix for chaotic microwave cavities with absorption was also experimentally investigated [63]. The distribution $P(R)$ of the reflection coefficient $R$ has been recently known for any dimensionless absorption strength $\gamma$ [64] and for systems with time reversal symmetry ($\beta = 1$) $P(R)$ was studied experimentally in [65]. Moreover, in the papers Hul et al. [25] and Lawniczak et al. [26] the distribution $P(R)$ of the reflection coefficient $R$ and the distributions of imaginary and real parts of Wigner’s reaction matrix $K$ for microwave networks with absorption were found using the impedance approach [57,58].

Figure 5 shows the experimental distributions $P(R)$ (squares) of the reflection coefficient $R$ for two mean values of the parameter $\gamma$, viz., 20.1 and 50.6. The experimental values of the $\gamma$ parameter were estimated for each realization of the network by adjusting the theoretical mean reflection coefficient $\langle R \rangle_{th}$ to the experimental one $\langle R \rangle = \langle SS^\dagger \rangle$, where

$$\langle R \rangle_{th} = \int_0^1 dRRP(R). \quad (11)$$

Figure 5 also presents the corresponding numerical distributions $P(R)$ (full lines) evaluated on the basis of the accurate formula given in [64]. A good
Fig. 5. Experimental distribution $P(R)$ of the reflection coefficient $R$ for the microwave fully connected hexagon networks for $\bar{\gamma} = 20.1$ (open squares) and $\bar{\gamma} = 50.6$ (full squares) [26]. The corresponding theoretical distribution $P(R)$ [64] for $\gamma = 20.1$ and $\gamma = 50.6$, respectively, is marked by the solid line.

Fig. 6. Experimental distribution $P(v)$ of the imaginary part of the $K$ matrix for the two values of the mean absorption parameter: $\bar{\gamma} = 20.1$ (open squares) and $\bar{\gamma} = 50.6$ (full squares) [26]. The corresponding theoretical distribution $P(v)$ [64] for $\gamma = 20.1$ and $\gamma = 50.6$, respectively, is marked by the solid line.
overall agreement of the experimental distributions $P(R)$ with their theoretical counterparts is seen.

In Figure 6 the experimental distribution $P(v)$ of the imaginary part of the $K$ matrix ($-v = \text{Im } K < 0$) is shown for the two mean values of the parameter $\bar{\gamma} = 20.1$ and 50.6, respectively. The experimental results in Figure 6 are in general in good agreement with the theoretical ones [26,64]. However, both experimental distributions are slightly higher than the theoretical ones in the vicinity of their maxima.

6.2 Elastic enhancement factor $W_{S,\beta}$

Microwave networks appeared to be very convenient for the experimental studies of the two-port scattering matrix $\hat{S}$ elastic enhancement factor $W_{S,\beta}$ [66,67]. The experiment was performed for microwave irregular networks simulating quantum graphs with preserved and broken time reversal symmetry in the presence of moderate and strong absorption [28]. In the experiment quantum graphs with preserved time reversal symmetry were simulated by microwave networks which were built of attenuators and coaxial cables connected by joints. Absorption in the networks was controlled by the use of microwave attenuators. In order to simulate quantum graphs with broken time reversal symmetry we used the microwave networks with microwave circulators. One should mention that the paper [68] has already reported a weak change of the enhancement factor due to partially broken time invariance in microwave cavity.

In the case of the two-port scattering matrix

$$\hat{S} = \begin{bmatrix} S^{aa} & S^{ab} \\ S^{ba} & S^{bb} \end{bmatrix}$$

(12)

the elastic enhancement factor $W_{S,\beta}$ is defined by the following relation [66,67]

$$W_{S,\beta} = \frac{\sqrt{\text{var}(S^{aa})\text{var}(S^{bb})}}{\text{var}(S^{ab})},$$

(13)

where $\text{var}(S^{ab}) \equiv \langle |S^{ab}|^2 \rangle - |\langle S^{ab} \rangle|^2$ denotes the variance of the scattering matrix element $S^{ab}$. One of the most important property of the enhancement factor $W_{S,\beta}$ for $\gamma \gg 1$ is connected with the fact that it should not depend on the direct processes present in the system [67,69].

In Figure 7 the enhancement factor $W_{S,\beta}$ of the two-port scattering matrix $\hat{S}$ of the microwave networks simulating quantum graphs with preserved and broken TRS, respectively, is shown as a function of the parameter $\gamma$.

The experimental results for the networks with preserved TRS (open circles) are in general good agreement with the theoretical ones predicted by [66,67]. Even for moderate absorption the experimental results are close to the theoretical ones. Because of absorption of microwave cables (network bonds) we could not test experimentally predicted by the theory [66,67] increase of the enhancement factor $W_{S,\beta=1} \rightarrow 3$ for very small values of the parameter $\gamma$. 
Figure 7 also shows that in the case of networks with broken TRS in the presence of moderate and strong absorption the experimental results (full circles) are in good agreement with the theoretical ones $W_{S,\beta}=2 \approx 1$ predicted by [66,67,69] within the framework of random matrix theory.

7 Conclusions

We demonstrated that quantum graphs with Neumann boundary conditions can be simulated experimentally by microwave networks. Undirected microwave networks simulate quantum graphs with time reversal symmetry. The results for the directed microwave networks with microwave circulators show that their characteristics such as the integrated nearest neighbor spacing distribution significantly differ from the RMT prediction for GOE, approaching the results characteristic of GUE. Therefore, directed networks can be used to simulate quantum graphs with broken TRS.

We also show that there are some spectral statistics, e.g., the second order level velocity autocorrelation function $c(x)$ that for larger fully connected Neumann graphs show deviations from the predictions of RMT for GOE. These parasite effects of localization can be minimized by use of COE graphs for which the autocorrelation function $c(x)$, in contrast to large Neumann graphs, shows very good overall agreement with the random matrix theory predictions.

Microwave irregular networks consisting of cables and attenuators are also very useful models of experimental systems with absorption. The experimental
results for the distribution $P(R)$ of the reflection coefficient $R$ and the distributions $P(v)$ of the imaginary part of Wigner’s reaction matrix obtained for microwave networks with absorption are in good overall agreement with the recent exact theoretical predictions for quantum systems with absorption [64].

The experimental studies of the enhancement factor $W_{S,\beta}$ of the two-port scattering matrix $\hat{S}$ for the microwave networks simulating quantum systems with preserved and broken TRS in the presence of absorption show good agreement with the theoretical predictions.

The results presented in this paper clearly demonstrate that undirected and directed microwave networks which simulate undirected and directed quantum graphs, respectively, can be successfully used to study large variety of wave phenomena predicted by quantum physics.

Acknowledgments. This work was supported by the Ministry of Science and Higher Education grant No. N N202 130239.

References

Evidence for Deterministic Chaos in Aperiodic Oscillations of Acute Lymphoblastic Leukemia Cells in Long-Term Culture

George I. Lambrou, Aristotelis Chatziioannou, Spiros Vlahopoulos, Maria Moschovi and George P. Chrousos

Abstract. Biological systems are dynamic and possess properties that depend on two key elements: initial conditions and the response of the system over time. Conceptualizing this on tumor models will influence conclusions drawn with regard to disease initiation and progression. Alterations in initial conditions dynamically reshape the properties of proliferating tumor cells. The present work aims to test the hypothesis of Wolfrom et al., that proliferation shows evidence for deterministic chaos in a manner such that subtle differences in the initial conditions give rise to non-linear response behavior of the system. Their hypothesis, tested on adherent Fao rat hepatoma cells, provides evidence that these cells manifest aperiodic oscillations in their proliferation rate. We have tested this hypothesis with some modifications to the proposed experimental setup. We have used the acute lymphoblastic leukemia cell line CCRF-CEM, as it provides an excellent substrate for modeling proliferation dynamics. Measurements were taken at time points varying from 24h to 48h, extending the assayed populations beyond that of previous published reports that dealt with the complex dynamic behavior of animal cell populations. We conducted flow cytometry studies to examine the apoptotic and necrotic rate of the system, as well as DNA content changes of the cells over time. The cells exhibited a proliferation rate of nonlinear nature, as this rate presented oscillatory behavior. The obtained data have been fit in known models of growth, such as logistic and Gompertzian growth.

Keywords: Proliferation, deterministic chaos, aperiodic oscillations, non-linearity, CCRF-CEM.

1. Introduction

The scope of the present work is to test the hypothesis posed by Wolfrom et al. that proliferation shows evidence for deterministic chaos. Biological systems are dynamic systems. The knowledge on how to determine a present state from the previous ones is critical within many areas, or applications, varying from cancer to insect population control. However, it has been proven a very tedious work to discover laws underlying biological systems, since on one hand it is not easy to model such systems due to their complexity, and on the other hand, biological dynamical systems posses significant adaptation capabilities. Their hypothesis was tested on adherent Fao rat hepatoma cells and it was found that these cells
manifest aperiodic oscillations in their proliferation rate, giving evidence for deterministic chaos. We tested this hypothesis, adding specific modifications to the previously published experimental setup. We used the acute lymphoblastic leukaemia cell line CCRF-CEM since it provided an excellent substrate for modelling proliferation dynamics. Several studies have been occupied with the complex dynamic behaviour of animal populations [1-4]. However, very little is known about the dynamics of tumour cell proliferation [5] and even less is known about the state of proliferation dynamics during oncogenesis; that is until cells reach an adequate population to be diagnosed. The data that can be collected from tumours, regarding their dynamic nature, can only happen after a tumour has been diagnosed, which usually is too late for the patient, as all the progress-determining steps have taken place. Therefore, in vitro systems provide an excellent opportunity to study effects that are impossible to measure in vivo. Most importantly, they enable the study of long-term behaviour, which is required when it comes to reaching conclusions with regards to non-linearity and chaotic system behaviour. This, in particular, is impossible to happen, even with primary cultures of cells, since they are short-lived (15-20 days) when untransformed, and the only way is the use of established cell lines obtained from different organisms. For that reason we developed a modelling approach so as to simulate the in vivo conditions as best as possible. Cells were seeded at a low initial concentration of 20 cells/µl. Since they grew in suspension we assumed that they reached an even/equal distribution in the media solution. Measurements were taken at least at two-day intervals, thus obtaining more than 80 measurements in total, exceeding the Wolfram et al. protocol, which took around 40 measurements. Also, taking a sample from a liquid culture has minimum effects on the total cell population, since it is not essential to trypsinize in order to take the sample; trypsinization, a requirement for obtaining samples from adherent cell cultures, stresses the cells and changes their proliferation dynamics. Cells were passaged at regular intervals. This practically removed the dead cells from the system and the remaining cells were allowed to grow again in a fresh medium. This allowed modelling of the growth of a tumour, such as leukaemia, in a space with finite capacity. Removal of cells modelled the circulation that removes dead cells from a particular position in the organism. Cells were grown for approximately 150 days (5 month period) while as previously reported, Fao cells were kept in culture for 200-240 days in total. The nature of proliferation dynamics may give insight into the way that cells not only proliferate but also differentiate.

2. Materials and Methods

2.1. The CCRF-CEM cell line:
The CCRF-CEM (T-ALL) cell line was used as the model, obtained from the European Collection of Cell Cultures (ECACC, United Kingdom). The CCRF-CEM cell line, a CD4+ [6] and CD34+ presenting cell line [7], was initially obtained from the peripheral blood of a 2 year old Caucasian female. She was diagnosed with lymphosarcoma which progressed to acute lymphoblastic leukaemia later on [8]. The child underwent irradiation therapy and
chemotherapy prior to obtaining the cell line. Although remission was achieved at various stages, the disease progressed rapidly.\[8\] The cell line has been observed to undergo minor changes after long-term culture, except for the presence of dense granules in the nucleoli.\[9\] Finally, the CCRF-CEM cell line has been reported to manifest autocrine catalase activity, which participates to its mechanisms of growth and progression.\[10\].

2.2. Cell culture conditions: Cells were grown in RPMI-1640 medium, 10% FBS and 0.1× Streptomycin/Penicillin at 37 °C, 5% CO₂ and ~100% humidity. Cells were cultured in 75cm² in total medium volume of 25ml. Cells were seeded at an initial concentration of 20 cells/µl and ~200 cells/µl and were fed at regular intervals thereafter. Medium changes took place by centrifugation at 1000 rpm for 10min, the supernatant was discarded and the remaining cells were rediluted in 25ml media and were allowed to grow.

2.3. Measurements, experimental setup and model: The CCRF-CEM cells grow in suspension and therefore give an excellent model of avascular growth. In addition, the following assumptions have been made for its proliferation: a) extracellular signal transduction takes place autocrinally, b) the cell distribution at seeding and thereafter is considered to be uniform and c) nutrient supply was considered to be stable since cells were fed at regular time intervals. All measurements have been performed in triplicates.

\textit{Wolfrom and collaborators (2000)}, had counted the cell population at the end of a time period varying from 5 to 7 days. At the end of this period, cells were trypsinized, measured and then seeded at an initial concentration of $10^5$ cells per flask.

In the present study, before every measurement, flasks were gently shaken in order to assure that the sample taken consisted of a representative, equally distributed population size. For the growth dynamics study of the cell culture system, an experimental setup was developed, where cells were assayed at least every 48h and the media renewed every 3-5 days. For the measurements, 200µl from each flask was taken and measured with a NIHON KOHDEN CellTaq-α hematology analyzer. In that way more than 80 measurements were obtained in a period of 150 days (5 months).

2.4. Mathematical model and analysis: We used a one-dimensional representation based on the assumption that the present state of our system is dependent upon the previous one. So, our system is better described by the logistic equation, as $f(x_{n+1}) = kx_n(1-x_n)$ (1) and with respect to time $\dot{x}_n = kx_n(1-x_n)$ (2) (the logistic differential equation). Both equations belong to the family of logistic equations of the form $f(x) = kx(1-x)$ (3), where $k$ is the proliferation constant. For the analysis of the data collected we have utilized phase-space and return maps and used the geometrical representation proposed by \textit{Wolfrom et al (2000)}. In addition, we have tested the dependence on initial conditions by using two different starting population sizes. For testing the
chaotic behavior of the system, we have calculated the Lyapunov exponent and searched for strange attractors or sources. Many methods have been proposed for the calculation of Lyapunov exponents and it is considered to be a difficult task \cite{11, 12}. In our case, given the function which we have based our model on, we used for the approximate estimation of Lyapunov parameters the following definition: Let \( f \) be a smooth map on \( \mathbb{R} \). The Lyapunov number \( L(x_1) \) for the orbit \( \{x_1, x_2, \ldots, x_n\} \) is defined as

\[
L(x_1) = \lim_{n \to \infty} \left( f'(x_1) \cdots f'(x_n) \right)^{1/n}
\]

(4) if the limit exists. In conjunction, the Lyapunov exponent \( h(x_1) \) is defined as

\[
h(x_1) = \lim_{n \to \infty} \frac{1}{n} \left( \ln |f'(x_1)| + \cdots + \ln |f'(x_n)| \right)
\]

(5).

3. Results

We have studied the proliferation dynamics of an acute lymphoblastic leukaemia cell line by developing a modelling approach, where cells from two different initial populations were allowed to grow with a periodic nutrient supply in order to sustain cell growth.

The time series produced from the experimental data showed a characteristic logistic pattern as described in (1), whereas proliferation rate with respect to time manifested an aperiodic oscillatory behavior (Fig. 1A and 1B). In fact, proliferation rate appears to manifest a saltatory pattern where cells after a period of “adjustment” to the environment start dividing rapidly. This was the first evidence that the dynamics of cell population can manifest complex behavior. Interestingly, when calculating the Lyapunov exponent of the two curves starting from different initial conditions, these gave different results (Fig. 2A). For the curve describing cell proliferation from 20 cells/ul, the Lyapunov
exponent $h$ was calculated to be >0, whereas for the curve describing cells starting from 200 cells/ul it was <0. Furthermore, for the orbit Lyapunov exponent was 0.13 for $x_0=20$ and -0.09 for $x_0=200$. The next criterion we investigated was whether the state-space manifested an asymptotically periodic pattern or not. Space-space representation has been proposed by Lorenz [13] and has been used by others in biological time-series [14]. State-space maps showed that irrespectively of the initial population (either 20 cells/ul or 200 cells/ul) both curves converged after a long period of cell culture (Fig. 2).
performed a Fast Fourier Transformation (FFT) analysis (data not shown) which did not show the prevalence of noise. On the other hand, how does nonlinearity emerge? The logistic equation, on which we based our model, assumes that a population grows and then decays due to a limited amount of nutrients. In our model this was not the case since we kept a constant supply of nutrients in order to keep cells growing. This led us to the conclusion that the nonlinear factor was not the population per se but rather the proliferation constant $k$. In our initial assumptions we assumed that nutrients were abundant and constant, whereas the changing environmental factor was space for growth. Space becomes limited, as time progresses, activating inhibitory mechanisms for growth. Therefore, when drawing the populations at time $t_n$ and $t_{n+1}$ as a function of the proliferation rate (which is equal to $f'(x)$ for discrete time points) we observed that although the system converges towards its possible steady-state it manifests nonlinear behavior (Fig. 2B, 2C). Therefore, we analyzed the proliferation rates calculated for each discrete point in the same way. In other words, we used the return map of the proliferation rates, the first derivative of the proliferation curve at each discrete point. So, let $k_n=\{f'(x_0), f'(x_1),...,f'(x_n)\}$ and $k_{n+1}=\{f'(x_1), f'(x_2),...,f'(x_{n+1})\}$ where $k$ is the proliferation rate from equations (1) and (2). $K$ can also be written as $\frac{dX}{dt}$ and $\frac{dX}{dt}+1$ for $t$ at $n$ and $n+1$ respectively with $n \in \mathbb{N}$ as presented in Figure 3B. Interestingly, drawing $k_n$ as a function of $k_{n+1}$ gives us a curve with at least two fixed points for both initial cell populations indicating a period-3 orbit (Fig. 3A). This period-3 orbit implies chaos as it has been previously reported [15].

4. Conclusion

It has been reported previously that biological systems exhibit very complicated dynamics [3, 5]. The present work addressed the question as to whether chaotic dynamics could be detected in the proliferation of acute lymphoblastic leukaemia cells in long-term culture. This had been proposed previously for adherent cell lines [5]. To the best of our knowledge no reports have been published on the proliferation dynamics of suspension cell cultures and in general studies on proliferation dynamics in vitro are scarce. The question that arises at this point is whether such studies are meaningful, since in vitro systems represent in vivo systems only in part.

In vitro systems offer the capacity of performing long-term studies, and isolating the system under study to reduce noise, both of which are not possible in in vivo systems. Cell cultures in vitro are considered to manifest a linear pattern of growth. Given the fact that the logistic equation takes into account limited nutrients and space, it predicts that a cell population would reach a steady-state within a certain time and eventually die out.

We have introduced a new constant to our model by making nutrient readily available but keeping space, in terms of total volume, constant. Under these conditions we draw the proliferation curve, which shows aperiodic oscillations,
whereas the proliferation rate manifests these aperiodic oscillations most clearly. As it was shown in Fig. 2A, the return map of Fig. 1A gave an almost perfectly linear function, where a “bell-shaped” geometry was expected.

However, when we expanded our analysis to the return map of proliferation rate (Fig. 3B) we observed a nonlinear behaviour and we found geometrically that the fixed points on this curve manifest a period-3 orbit (Fig. 3A) which implies chaos dynamics. Our work shows evidence for deterministic chaos in the proliferative behaviour of leukaemia cells in vitro. Since this is a very complicated phenomenon it requires a lot more effort to understand the mechanisms underlying those dynamics. The implications from the understanding of these systems are tremendous. It will give us insight to the mechanisms of disease progression, such as in cancer, and enable building advanced models for the disease, which combine important features of both in vitro and in vivo systems. It is known that cancer starts and progresses slowly, at least before clinical presentation. Knowledge on the mechanisms of growth before the clinical symptoms become obvious may contribute to the early treatment of this and other diseases.

References


Dynamical Systems, Mimesis, and Analogy in Experimental Music

Scott Mc Laughlin

University of Huddersfield, UK
(E-mail: s.mclaughlin@hud.ac.uk)

Abstract. Music and dynamical systems share aspects of patterning, repetition, and variation over time, but most music that references dynamical systems as a compositional influence are mimetic representations of the system, the music is a static 'snapshot' of the system. I propose an approach where the compositional and performative processes are analogous to the dynamical system, and the music develops in realtime through performance, acting as a model of the system in musical form. The dynamical system process is translated from the mathematical to the musical/performative, retaining its mechanisms but in a new medium. This paper will explore two examples of previous mimetic approaches, and a brief exposition on similarities between dynamical systems and musical indeterminacy (in experimental music). I will then present examples from my work There are Neither Wholes Nor Parts (2011), showing how feedback and hysteresis are used to create musical processes that affords non-linear and emergent sound structures.

Keywords: hysteresis, feedback, composition, music, improvisation.

1 Background and Definitions

Non-linearity and chaos are exciting ideas for composers in many ways. Music is essentially patterns of repetition and variation over time, and much of musical structure and meaning is predicated on the ambiguities of tension and release (see [6]). Non-linear systems such as strange attractors are intrinsically musical because they hover between variation and repetition, defining a structure gradually over time. Well-known examples of composers taking inspiration from dynamical systems include Ligeti’s Piano Études (1985), which reference self-similarity and fractals in relation to the development of rhythm and pitch cells through the piece. Danish composer Per Nørgård also turned to fractals as the inspiration behind his “infinity series” technique, saying:

Chaos is fascinating because you have an order behind chaos and chaos behind order. That fits very well with my feeling of life too[1].

Ligeti and Nørgård’s inspiration is a version of an ancient theme in Western Art, that of “unity”, a deeper order behind a seemingly chaotic surface (see
These composers’ works are examples of poetic inspiration, where the idea of dynamical systems can be applied to a composer’s musical language, generating a musical idea from a non-musical source. Section 2 examines in more detail the mimetic aspect of making music from dynamical systems.

I would like at this point to make a distinction between dynamical systems used in computer music and acoustic music. For this paper I will refer only to acoustic music, primarily because the use of dynamical systems in computer music is a healthy discipline with many fine examples of the realtime sonification of dynamical systems (see section 2), whereas I am proposing the application of dynamical systems to acoustic music in a manner that goes beyond the poetic, in which the dynamics of the system must be analogised in order to make it performable. I believe my research in this area represents tentative steps in a hitherto unexplored area with much potential for future work.

2 Mimesis, analogy, sonification

The generation of composers active when chaos theory was first popularised adopted it largely from a mimetic perspective, where the objects and structures of chaos theory are used to inform the composition of linear musical structures. The music is not literally mimetic, in the sense that the composers are not intending to imitate or represent what inspires them, rather the inspiration leads a musical idea, translating the physical into musical language. This translation can take the form of a highly poetic inspiration, or a more literal sonification, I present examples of both below.

2.1 Poetic mimesis

In Tristan Murail’s *Attracteurs Étranges* (1992) for solo cello, he describes his use of the strange attractor as a “poetic analogy”:

The melodic contours of the cello describe spirals that always seem to return to one of several identical points, but in fact always follow differing, warped or diverted trajectories.[7]

Murai takes a mimetic approach, translating the “warped trajectories” of the attractor into a musical language and composing a piece which is a static and linear representation of the dynamical system, like a musical photograph of the attractor, fixed and unchanging. Of course if should be noted that in live performance the piece will be “dynamic” by virtue of its unfolding in realtime, but this is still in reference to the fixed score, the dynamical system is not mapped in a manner that allows the piece to change each time it is performed.

For my argument, the terms “computer music”, “electronic music”, and “electroacoustic music” are essentially interchangeable, encompassing any musical situation where the computer is used for sonification of data in realtime.
2.2 Sonification

Sonification is a more rigorous approach to translation, where the equation or resulting data is mapped—directly or indirectly—onto some parameters of sound. Michael Winter defines sonification as follows:

The parametric profiles of the changing characteristics of sound can be expressed as mathematical functions of time. By using physical scenarios and mathematical functions to determine these parameters, one can distance oneself from aesthetic opinions and attempt to relinquish intuition. This provides another way to create a new music.[13]

Outside the domain of electronic music, Iannis Xenakis is the composer most associated with the mapping of scientific and mathematical concepts onto musical parameters. His biographer Nouritza Matossian has this to say about Xenakis’ sonification of such ideas:

Xenakis never claimed that a rigorous mathematical basis is sufficient to produce a well-formed piece of music. Those who are partially informed about the mathematical theory expect the music to be a mirror of mathematical processes and equations. *Pithoprakta* is no more a translation of probability theory than an artichoke or a celery is a translation of the Fibonacci series, or a flowing river is a translation of random functions. [...] Even though underlying structures are shared, particularity of musical resources ensures uniqueness in each one.[5]

Sonification is another way of interpreting non-musical information through sound in a way that allows the structures in that information to be made audible.

A brief note about musical notation. In computer music, sonification generally means bypassing the symbolic layer of notation. For example, taking realtime data from a weather satellite and mapping it to pitch/duration/etc. requires no notation other than the necessary code, which is interpreted somewhat literally (by the computer). In acoustic music, musical notation is usually a required step to interface with the performance traditions of musicians, and the interpretation of that notation is subjective; different performance traditions establish competing authoritative versions of practice. Transforming data into notation inevitably involves some scaling to appropriate ranges, but more problematically it can also involve the quantisation of data to fit musical scales and rhythmic durations. Such quantisation is only problematic from the point of view that the musical result may be less musical but more interesting without it. This is not to say that the music has to be “true” to the data, to be understood it should be translated in a manner that is idiomatic to the styles and languages of the new medium. However, much of the interest in this sort of cross-breeding of ideas is that new processes and languages can emerge, by trying too hard to fit the traditional clothing of music, this can be lost.

As an example of sonification in acoustic music, in Rolf Wallin’s *Onda di Ghiaccio* (1989), “fractal equations are applied to the musical materials to describe the dynamics of a turbulent process”[12]. Wallin uses a “symmetrically
coupled nonlinear system” to generate stochastic maps which control musical field parameters such as pitch center, pitch range, field duration etc., thus the dynamical system creates a fixed scaffold onto which the musical detail is composed: see also Wallin[10] for a more detailed explanation of the mapping. This is less mimetic than the Murail example but still a static representation of a dynamic process. In these examples the motion of the turbulent process is only imitated by the flow of the music, both of these applications are compositional devices that mimic their respective dynamic processes. That said, I'm sure both composers would be at pains to point out that the dynamical system here is inspiration for a musical structure, the mimesis is not intended to be literally representative of the system. As Wallin states:

This is my first attempt to use fractal mathematics in my music. The Italian title (“Icewave”) emerged in the very end of the creation of the piece, and is only one of many possible titles describing a turbulent motion captured - or frozen - in a specific moment. The notion of a wave stretched out to last 12 minutes has nothing to do with sound imitation. Instead I try to describe the dynamics of every turbulent process, be it in water, air or for that matter in our lives, where order, chaos, predictability and unpredictability give way for each other in an ever changing pattern.[11]

Both the Murail and the Wallin pieces are examples of approaches to using static snapshots of dynamical systems as a model for composing linear music. My research is not intended as a replacement for the above approaches, or to invalidate them, rather as another way of approaching dynamical systems that is less static. In the following section I will show how indeterminacy is used in experimental music to create pieces that are not static or linear, and in section 4 I will show how the tools developed by experimental music composers in can be integrated with dynamical systems as models for composition of non-linear music.

3 Experimental music, Indeterminacy and dynamical systems

For clarity, it should be explained that Experimental Music is a very broad genre, and by no means all of it conforms to my description below. There are many ways of challenging musical traditions and asking the question “what can be music?”, but I wish to focus here on music that challenges received ideas of structuring, teleology, and linearity in music. Also, the music described below does not use dynamical systems as a model, but it is in many ways a more dynamical music than traditional score-based Western music, and as such I use it to demonstrate my own compositional heritage and the existence of a modern music that eschews linear construction.

The paradigm of indeterminacy, as used in Experimental Music, is demonstrably non-linear in a musical context, either as compositional process (such as Cage’s “chance” procedures) or as a performance-based process (in the music of
Christian Wolff, Cornelius Cardew, *et al*). The non-linear structures of strange attractors and other chaotic objects can be applied to indeterministic musical processes to move beyond the linear paradigm of static musical structures into the realm of dynamic structures and material. John Cage describes a goal of art as to “imitate nature in the manner of her operation”[4]. What I propose is analogy rather than mimesis as compositional process, where the process is translated from the mathematical to the musical/performative, retaining the mechanics but in a new medium.

In the 1960s, John Cage’s popularisation of the concept of indeterminacy in music was in large part responsible for the formation of the school of experimental music, which I would describe as a schism in the composition and performance of Western music, and more importantly, a sea-change in how music is listened to. Among other things, experimental music expands on Duchamp’s ideas of Art by drawing attention to the audient as an active rather than passive participant. In the case of music this is an acceptance that music is an esthesic process. The prevalent model of pre-experimental music was the narrative—in “pure” formal music as well as in programmatic music—that led the listener through a journey of the composer’s design, a mainly linear experience. In much experimental music the model shifts to an experiential one, where the listener is presented with an environment that unfolds in time, a significantly less linear music.

Leonard Meyer, in his theories of meaning and emotion in music (see [6]), describes meaning in information-theoretic terms, as a function of the predictability of the musical structure based on its moment-by-moment development. In his analysis, well-composed music manipulates a sweet-spot in the human perception of musical repetition and variation, wherein the music changes just enough to be interesting but not so much that it alienates or bores the listener. In a linear piece of music this is generally controlled by the composer, working to a traditional sense of musical proportion (where the music should climax, or rest, etc.) in order to create a teleological experience and lead the listener through a narrative structure (whether explicit or implicit). In Experimental Music it is more often the case that strict linear structuring is replaced with a field-model, where musical materials are presented in time as co-existing objects without explicit relationships. Structure in Experimental Music is thus often a function of the listener’s experience, rather than an explicit structure of the composer’s design.

Looking at how indeterminacy is used in music, Cage’s own strategy was mainly pre-compositional, in that he would employ randomisation—rolling dice, consulting the *I Ching*, or even using imperfections on the surface of the paper to decide on positions of notes on the stave—in the choice of notes and more: his concern was to distance himself to some degree from the compositional act, to make it less about ego and control, and to “let the sounds be themselves”[4]. These works are created using indeterminacy but are still largely linear in performance.

To create less linear works, many composers experimented with pieces where sections of music with fixed notation can be played in any order, locally linear but globally non-linear; for example, Stockhausen’s *Klavierstück XI from*
1956[9]. However, truly non-linear music requires not just the structural sections but the musical material itself to be indeterminate at some level. Approaching this ideal is the music of Christian Wolff, which often allows the material to be chosen by the performer, with Wolff specifying types or sometimes only specifying abstract or poetic relationships between events/materials. Wolff includes elements of feedback in his work by encouraging listening among players, and suggesting (not instructing) that they take cues from each other: the socio-political impetus behind this is give the players more choice and independence, an act of resistance against the control structures of much Western music. In works such as *Burdocks* (1970-71) and *Changing the System* (1972-73), he makes the temporal aspect of the music dependent on the interaction of the players by using cueing systems rather than the traditional grid of beats and bars.

Wolff’s piece *Edges* (1968) is especially non-linear. The score lays out a series of symbols scattered arbitrarily on a page, with a corresponding legend to explain the symbols. The performers are not to play the symbols themselves, but rather use them as points to be approached. Wolff explains in the score:

> [the symbols] mark out a space or spaces, indicate points, surfaces, routes or limits. A player should play in relation to, in, and around the space thus partly marked out. He can move about in it variously (e.g. in a sequence, or jumping from one point to another), but does not always have to be moving, nor does he have to go everywhere. Insofar as the signs are limits, they can be reached but should not be exploited. The way to a limit need not be continuous, in a straight line.[14]

The piece is non-linear in its approach to time, there are no suggestions, symbolic or textual, as to how long the piece or any individual event should last. The player moves between events as they choose, in no fixed order. Yet the piece still has a structure, a set of “limits” to be approached by the players, and the interactions between these players as they influence each other, a subjective sort of feedback. The piece is also non-linear in its interpretive space. Each symbol is asymptotic in relation to its interpretation. Some are subjective, the symbol “very rapid” can be approached up to the physical limits of the player, but the limit itself is inexact. Some are more literal, “directly after a long sound” is a very clear instruction but there are an infinity of ways to play not—“directly after a long sound” and still be approaching this limit.

Experimental music has developed many notational and performative techniques for creating non-linear music. As a composer I have taken these techniques and developed them to include elements of feedback in order to take advantage of the structuring aspect of dynamical systems. In the following section I outline a recent example and the method used.

4 **Hysteresis as compositional/performative process**

In my compositional research, the series of pieces titled *There are Neither Wholes Nor Parts* (2011) uses feedback and hysteresis to generate musical
structures in realtime through the interaction of two elements: (1) the score (a notation and set of interpretive rules) that drive the performer’s pitch choices; (2) and the non-linearities of the woodwind multiphonics that make up the material of the piece: these pieces are written for woodwind instruments using only multiphonics. This section explains the choice of multiphonics as musical material, and how feedback has been used in the compositional method.

Multiphonics are used in this piece because the sound is interesting to me as a composer, but also because they have a non-linear response and produce frequencies outside the standard tempered scale of musical pitches. Arthur Benade describes multiphonic oscillation as:

a collection of components whose frequencies are connected to one another by an elaborate set of heterodyne relationships. The ordinary tones of woodwind instruments also fit this description, but the frequency components in normal tones are limited to those belonging to a single harmonic series.\[2\]

Multiphonics are generally perceived as a complex sound made up of two or more notes, and the difference/combination tones resulting from the interaction of the multiple superimposed air columns. Botros et al cite Backus as reporting that “the heterodyne components from the interaction, [indicate] a non-linear super-position of the two notes.”\[3\] These non-linear relationships mean that multiphonics are relatively unstable and unpredictable in performance, requiring specialist knowledge of the musician to control them and make the performance viable. In these pieces, the performer is asked to play full multiphonics, and also to isolate individual partials (using breath pressure and embouchure), as well as some in-between states: see Figure 1. Specific multiphonic fingerings can also exhibit considerable variability in pitch results across different players and instruments, so for my compositions I have avoided any references to specific fingerings, instead the performer uses whichever multiphonics work best for them as material for the performance, while the score defines the musical relationships that the performer should create with this material. This non-specificity of material is a common approach in experimental music.

To explain the feedback mechanism, it is important to understand that the same perceived pitch in a multiphonic can be achieved using different fingering configurations on the instrument. However, different fingerings produce differences in harmonic spectra, and even multiphonics that sound similar in pitch have small deviations in specific frequencies of partials: see Figure 2 for comparative sonograms of two different multiphonic fingerings. These compositions rely on these small deviations because the most important instruction in the score is for the performer to try to keep the strongest perceivable pitch in the multiphonic the same from event to event. This is countered by the score this terminology is inaccurate but for the purpose of my argument it is sufficient to distinguish between playing the full spectrum of the multiphonic and isolating individual pitches from that complex spectrum. Figure 1 shows that single partials are not always isolated, sometimes a single harmonic series is isolated, but to the listener these differences are quite subtle.
Fig. 1. Sonogram of a single multiphonic showing progression from an isolated partial to the full multiphonic and ending on a different isolated partial: like event C in Figure 3.

also requiring the performer to constantly change fingerings, and play different phrase-shapes: such as moving from a single partial to a full multiphonic on the same finger. For example, a certain fingering may produce the correct frequency but may not allow that frequency to be isolated as a single partial, so it may not be possible to use that fingering in certain events (see Figure 3 for some events with different phrase-shapes). The dialectic of the music is that the score pushes the performer in two contradictory directions simultaneously, the forward motion of moving through the space of available fingerings, and the reverse motion of keeping each pitch as close as possible to the previous. The musical result is a structure straining to maintain a pitch identity, with the occasional but inevitable abrupt shifts to a new pitch area when the performer finally runs out of options.

Figure 3 shows a section of the score for *There are Neither Wholes nor Parts* 2 with three different events; separated by the double vertical lines. The first event, A, is initially a single sustained partial (isolated from a multiphonic), which in the second half of the event is joined by another partial of higher frequency: shown in parentheses to indicate that this should be barely audible, a ‘halo’. For event B the frequency of this ‘halo’ partial is carried across, this time as a single partial, with another ‘halo’ partial of lower frequency. In the second half of B after the breath mark (the comma) the situation is inverted. The final event, C, begins and ends with single partials, with a complete multiphonic between them. The text below A and B is the repeat instructions for each event: B is repeated three times, one of which must be a different fingering; C is repeated four times, two of which must be different fingerings.
Fig. 2. Sonograms of two different multiphonic fingerings that sound similar, showing how prominent partials are similar in frequency but small deviations in overall spectra are clear.

Fig. 3. Score example from There are Neither Wholes nor Parts 2.
The non-linearity of the music is due to the many possible paths that each event can take, and that these paths are all defined by the non-linear response of the instrument to multiphonic fingerings. For example, if event A is 440Hz, there may be ten fingerings that can produce that frequency, and be able to produce a higher frequency ‘halo’ partial as well, but each of these fingerings will produce a different ‘halo’ partial at a different frequency. Assume the player chooses a fingering with a ‘halo’ partial at 500Hz, this limits B to another group of potential fingerings, ones that include partials at or around 500Hz, and are capable of playing the phrase-shape of B with its inverted envelopes. There is also the repetition of B which requires a second fingering, one that includes all the above attributes, or as close as possible.

There are Neither Wholes nor Parts 2 has a musical structure that exhibits the standard attributes of repetition and variation over time, generated through interaction of materials and the feedback mechanism. The structure is dependent on initial conditions as each event is dependent on the last; a different starting frequency on a different instrument can radically alter the course of the piece. The piece is designed so that pitch is the defining factor in the perception of structure, and pitch is the element that has the most radical potential for variation over the course of the piece.

5 Conclusions

My initial research was undertaken from readings of popular texts on Chaos Theory, this gave me sufficient insight to generate compositional ideas that have taken the research this far, but it would be interesting to take the work further by collaborating with a researcher who understands dynamical systems at a deeper mathematical level.

This set of pieces is a early attempt to introduce mechanisms of feedback and hysteresis into music as a dynamical system. The mechanism used in There are Neither Wholes nor Parts has been successful both compositionally and in performance. The players who have taken on the piece have all found it to be a stimulating challenge to prepare the piece, and with time it will be interesting to see if they can also approach the piece without needing to create a fixed version, but instead simply react according to the what the instrument gives them.

The next step in this research is to write a piece for two instruments. This will provide more possibilities for feedback based on two states rather than one, and to use hysteresis based on the current position (pitch) of one relative to the other.

References

Influence of the simulation model on the spatial arc resistance distribution of an axially blown switching arc

Matthias Hoffacker, Paul G. Nikolic, Daniel Eichhoff, Andreas Kurz

Abstract: Circuit breakers are important elements of the electric power supply system. Due to the contact separation during the switch-off process an electric arc is ignited within the circuit breaker. A forced flow of the insulating quenching gas medium is used to cool the arc influencing its conductivity. Only if the power dissipation due to cooling exceeds the electrical power input by ohmic heating, the arc is extinguished and the current is successfully interrupted in its natural zero crossing (CZ). As the impact of the cooling by the quenching gas on the resistance of the arc is considered crucial for the success of the switch-off process, the spatial distribution of the resistance is of high importance for the assessment of a circuit breakers performance.

Research and development projects related to circuit breakers more and more often use computational fluid dynamics (CFD) simulations. The implemented simulation models have to be verified by adequate experiments. This paper deals with the influence of the simulation model on the simulated spatial arc resistance distribution near current zero. Different approaches for modelling the chaotic and turbulent phenomena of the arc are introduced and their results are compared with values measured in experiments. Here the turbulence model is of main interest. On the one hand the investigations show a good agreement between simulative and experimental results for the total arcing voltage when using adequate models. On the other hand these turbulence models lead to differences in the calculated spatial arc resistance distributions – which cannot be verified by experiments so far.

Keywords: CFD-simulations, circuit breaker, high voltage, arc, arc resistance, spatial resistance distribution, chaotic modeling, turbulence, turbulence model

1 Introduction

Circuit breakers are important elements of the electric power supply system. They are necessary for the safe switching of rated currents and the interruption of short-circuit currents. Today’s high voltage power supply system’s predominantly make use of self blast circuit breakers using sulphur hexafluoride (SF₆) as insulating and quenching gas. The contact separation during the switch-off process creates an electric arc within the circuit breaker. By cooling with a forced flow of the insulation medium the energy is dissipated until the arc is extinguished. Simultaneously the resistance of the arc rises. The value of the
resistance and its distribution along the arc is the crucial factor for the switch-off process to be successful [1].

Research and development projects related to circuit breakers increasingly use computational fluid dynamics (CFD) simulations as these simulations can reduce the number of cost-intensive reference experiments and allow the visualization of physical values which are not – or only very difficult – accessible in experimental investigations. Thus, they can also improve the understanding of the physical processes in the plasma of the electric arc during the switching operation of circuit breakers.

However, this paper deals with the influence of the simulation model on the calculated spatial arc resistance distribution near current zero. The arc resistance is mainly influenced by the convective and turbulent cooling of the quenching gas flow [2]. This leads to a non-linear arc resistance distribution near current zero. Hence, the simulation models need to consider both cooling mechanisms. Different approaches for modelling the turbulent phenomena of the arc are introduced and their results are compared with values measured in experiments.

Firstly experiments using a circuit breaker prototype are carried out. Here the arcing voltage close to the natural current zero (CZ) in the 50 Hz sinusoidal oscillation of the electric network is of main interest. Secondly CFD-simulations of the switching operation are performed using different turbulence models for the calculation. The results of these simulations are compared with the experimental ones.

2 Experimental investigations

For the experimental investigations the behaviour of a circuit breaker prototype is investigated in a synthetic test circuit.

Fig. 1. Cross-sectional view of the circuit breaker model used in the experiments
A cross-section of the test breaker is given in figure 1. The arc is ignited between the electrodes by a thin copper wire which evaporates due to the high current flow of more than 10 kA. The formed electric arc is burning inside the nozzle which is made of polytetrafluorethylene (PTFE) and evaporates material from the nozzle surface. This ablation and the heating by the arc lead to a pressure rise inside the nozzle which is relieved through the heating channel into the heating volume of the breaker.

As a consequence, the pressure in the heating volume rises accordingly. When the sinusoidal current and thus the power input by the arc decrease, the gas flow reverses and the quenching gas flow from the heating volume cools the arc inside the nozzle. If the cooling power of the quenching gas flow exceeds the power input of the arc the current can be interrupted during its natural current zero crossing.

For the experimental investigations in this paper a synthetic Weil-Dobke test circuit is used. The equivalent circuit diagram is shown in figure 2. The pre-charged capacitor \( C_T \) and the inductor \( L_T \) form a 50 Hz-resonance circuit together with the test breaker (TB). Closing the making switch (MS) and subsequently opening the auxiliary breaker (AB) one half period of a high current sinusoidal oscillation is precisely applied on the test breaker. The elements \( C_S \) and \( L_S \) form another resonance circuit, called injection circuit, with a frequency of approximately 950 Hz. This oscillation is triggered by the ignition spark gap (ISG) 500 µs before the end of the high current phase and causes a dielectric stress for the breaker after current interruption. The shape of this so-called transient recovery voltage is determined by the elements \( R_p \) and \( C_p \). For the measurement of the currents a Rogowski-coil and a coaxial shunt are used. Details on the Weil-Dobke test circuit can be found in [3].

Fig. 2. Equivalent circuit diagram of a synthetic test circuit after Weil and Dobke used for the experimental testing
3 Simulations

Computational-Fluid-Dynamic (CFD) simulations are a state-of-the-art tool in the development of high voltage circuit breakers, reducing the amount of time consuming and cost intensive experimental investigations. Nevertheless the applied simulation models need to be verified as the results of the simulation of a switching operation are sensitive to small changes in the geometry or the used models. The considered circuit breaker prototype used in the experiments is simplified for the simulations. This simplified geometry is given in figure 3. The 3-dimensional breaker prototype is replaced by a 2-dimensional, axis-symmetric model which is reduced to the region of interest – the arcing zone. The heating volume of the breaker is substituted by an inlet with the corresponding gas temperature, pressure and composition. Due to the fact that solely a time period of some µs before current zero is simulated these values are quasi constant. They are derived from simulations of the full high current period of 10ms. The applied mesh has its highest resolution in the area of the highest gradients of the physical values, i.e. along the axis of symmetry.

![Fig. 3. Geometry for the CFD simulations](image)

During the switching operation of a circuit breaker different physical phenomena occur. These are for example supersonic gas flows, turbulence, dissociation of the gas, radiation and ablation of the PTFE nozzle surface. They have to be considered in the CFD-simulation by using different models. Here the influence of the model for the calculation of the turbulence effects is investigated. The dissociation of the gas is considered by using appropriate gas data from look-up-tables providing transport and thermodynamic properties of the gas for pressures up to 100 bar and temperatures up to 40000 K. The radiation is calculated according to the discrete ordinate method (DOM) [4] and the model published in [5] is used to describe the ablation of the nozzle surface.

For predicting the effect of turbulence two different methods can be employed. Both calculate the mean gas flow parameters by using the Navier-Stokes equations. The first turbulence calculation method is based on the Reynolds Averaged Navier-Stokes equations and uses time averaging to predict the
turbulence effects. The turbulent fluctuations are calculated by means of modelling the kinetic energy \( k \) and the kinetic energy dissipation rate \( \varepsilon \). Therefore different approaches exist [4].

The second turbulence calculation method is based on a large eddy simulation and uses a spatial averaging of the Navier-Stokes equations and thus extends them by sub grid scale stresses. For modelling these sub grid scale stresses different approaches exist [4].

The energy balance of an electric arc differentiates between different physical effects and can help to understand the cooling processes during the switching operation. The current driven through the plasma in the circuit breaker by the electrical network causes the ohmic heating. The heating power per volume \( (p_{\text{ohm}}) \) can be calculated by knowing the electric conductivity \( (\sigma) \) and the electric field \( (E) \):

\[
p_{\text{ohm}} = \sigma |E|^2
\]

For the cooling of the arc by the gas flow from the heating volume different cooling mechanism are responsible. The three main effects are the cooling by radiation, by microscopic turbulence effects and the convective cooling. They can be calculated according to [6]:

\[
p_{\text{rad}} = \sum_{n=1}^{N} \sum_{m=1}^{M} \nabla \cdot \left( I_n w_m s_m \right)
\]

\[
p_{\text{turb}} = -\frac{\partial}{\partial x} \left( \lambda_x \frac{\partial T}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \lambda_r \frac{\partial T}{\partial r} \right)
\]

\[
p_{\text{conv}} = \rho \left( u \frac{\partial h_0}{\partial x} + v \frac{\partial h_0}{\partial r} \right)
\]

It is known that the effectiveness of these cooling effects depends on position and time [6]. Thus it might occur that the radiative cooling dominates in one part of the arc while the turbulent cooling dominates in another part. These differences can be visualized in CFD-simulations. However it is not possible to separate between the different cooling mechanisms in experimental investigations. To be able to verify the results of the CFD-simulations by experiments anyhow, the spatial arc resistance distribution has to be determined. The arc resistance is depending on the temperature of the plasma and thus on the local power balance.
Hence the arc resistance distribution is an indication for the local cooling power. As the conductivity and the electric field are coupled by the electric current density ($J$) by

$$\sigma = \frac{J}{E},$$

the electric field can be used to visualize the spatial cooling power.

4 Results

Up to now experiments can only provide information on the total arcing voltage – not on their spatial distribution. Typical shapes of measured current and voltage are given in figure 4. The high current phase lasting until 11 ms is then superpositioned with the injection current. The region of interest ranges from the last increase of the arcing voltage at approximately 11.5 ms to the final extinction of the current flow. The typical arcing voltages at $t = 1\mu$s (CZ at $t = 0$) are in the range of $U = 750...1300$ V.

Fig. 4. Exemplary current (black) and voltage (red) shape for an experiment

To analyze the local cooling power of the quenching gas flow in the CFD-simulations the electric field along the axis of the arc – which is proportional to the local arc resistance – is plotted. The black curve in figure 5 shows the behaviour without any turbulence model. One can see that the cooling power is highest in the centre of the nozzle where a stagnation point occurs due to the radial symmetric gas flow. The red curves in the same figure show the electric field for simulations using the k-ε-turbulence model with three different parameters (P1-P3). This model predicts high turbulence in the outer parts of the
nozzle. Thus an increased arc resistance and an increased electric field are observed. By using different parameters for the model the general shape remains constant while its height can be influenced. The total arcing voltage is derived by integration of the electric field along the axis of the arc and is given in the legend of figure 5.

Fig. 5. Electric field along the axis of symmetry for simulations without turbulence model and simulations using the k-ε-turbulence model with different parameters at \(t=1\mu s\)

Fig. 6. Electric field along the axis of symmetry for simulations using different turbulence models at \(t=1\mu s\)
In addition CFD-simulations are carried out using the following different turbulence models: RNG-k-ε, Kato-Lauder k-ε, k-ω, Low Reynolds (Chien) and Large Eddy. Their results are plotted in figure 6. While the simulations using the RNG-k-ε and the k-ω turbulence models lead to results comparable to the simulation without turbulence model the result of the Kato-Lauder k-ε model is comparable to the simulation using the standard k-ε model. The large eddy model predicts the highest cooling power in the region left and right of the stagnation point. Here the electric field strength is higher than in all other simulations.

5 Conclusions

In the experiments of this contribution the arcing voltage of a self blast circuit breaker prototype shortly before current zero has been investigated and compared to CFD-simulations using different turbulence models. The simulated total arcing voltage is within the variation of the experimental measured voltages at \( t = -1 \mu s \) before current zero. But depending on the applied turbulence model and its parameters the predicted arc resistance distributions – visualized by plotting the electric field – significantly differ.

Using state-of-the-art measurement technology the simulated resistance distribution cannot be verified in a real circuit breaker experimentally. Hence, future research aims for the development of a new measurement technology to determine the spatial arc resistance distribution from experiments providing a deeper insight into the physical cooling processes of blown switching arcs.

References


Particle based method for shallow landslides: modeling sliding surface lubrication by rainfall

Emanuele Massaro¹, Gianluca Martelloni¹,², and Franco Bagnoli¹

¹ Department of Energy "Sergio Stecco", University of Florence, Italy
(E-mail: emanuele.massaro@unifi.it, franco.bagnoli@unifi.it)
² Earth Sciences Department, University of Florence, Italy
(E-mail: gianlunca.martelloni@unifi.it)

Abstract. Landslides are a recurrent phenomenon in many regions of Italy: in particular, the rain-induced shallow landslides represent a large percentage of this type of phenomenon, responsible of human life loss, destruction of assets and infrastructure and other major economical losses. In this paper a theoretical computational mesoscopic model based on interacting particles has been developed to describe the features of a granular material along a slope. We use a Lagrangian method similar to molecular dynamic (MD) for the computation of the movement of particles after and during a rainfall. In order to model frictional forces, the MD method is complemented by additional conditions: the forces acting on a particle can cause its displacement if they exceed the static friction between them and the slope surface, based on the failure criterion of Mohr-Coulomb, and if the resulting speed is larger that a given threshold. Preliminary results are very satisfactory; in our simulations emerging phenomena such as fractures and detachments can be observed. In particular, the model reproduces well the energy and time distribution of avalanches, analogous to the observed Gutenberg-Richter and Omori distributions for earthquakes. These power laws are in general considered the signature of self-organizing phenomena. As in other models, this self organization is related to a large separation of time scales between rain events and landslide movements. The main advantage of these particle methods is given by the capability of following the trajectory of a single particle, possibly identifying its dynamical properties.

Keywords: Landslide, molecular dynamics, lagrangian modelling, particle based method, power law.

1 Introduction

Predicting natural hazards such as landslides, floods or earthquake is one of the challenging problems in earth science. With the rapid development of computers and advanced numerical methods, detailed mathematical models are increasingly being applied to the study of complex dynamical processes such as flow-like landslides and debris flows.
The term landslide has been defined in the literature as a movement of a mass of rock, debris or earth down a slope under the force of gravity [1,2]. Landslides occur in nature in very different ways. It is possible to classify them on the bases material involved and type of movement [3].

Landslides can be triggered by different factors but in most cases the trigger is an intense or long rain. Rainfall-induced landslides deserved a large interest in the international literature in the last decades with contributions from different fields, such as engineering geology, soil mechanics, hydrology and geomorphology [4]. In the literature, two approaches have been proposed to evaluate the dependence of landslides on rainfall measurements. The first approach relies on dynamical models while the second is based on the definition of empirical rainfall thresholds over which the triggering of one or more landslides can be possible [5]. At present, several methods has been developed to simulate the propagation of a landslide; most of the numerical methods are based on a continuum approach using an Eulerian point of view [6,7].

An alternative to these continuous approaches is given by discrete methods for which the material is represented as an ensemble of interacting but independent elements (also called units, particles or grains). The model explicitly reproduces the discrete nature of the discontinuities, which correspond to the boundaries of each element. The commonly adopted term for the numerical methods for discrete systems made of non deformable elements, is the discrete element method (DEM) and it is particularly suitable to model granular materials, debris flows and flow-like landslide [8]. The DEM is very closely related to molecular dynamics (MD), the former method is generally distinguished by its inclusion of rotational degrees-of-freedom as well as stateful contact and often complicated geometries. As usual, the more complex the individual element, the heavier is the computational load and the “smaller” is the resulting simulation, for a given computational power. On the other hand, the inclusion of a more detailed description of the units allows for more realistic simulations. However, the accuracy of the simulation has to be compared with the experimental data available. While for laboratory experiments it is possible to collect very accurate data, this is not possible for real-field landslides. And, finally, the proposed model is just an approximation of a much more complex dynamics. These arguments motivated us in exploring the consequences of reducing the complexity of the model as much as possible.

In this paper we present a simplified model, based on the MD approach, applied to the study of the starting and progression of shallow landslides, whose displacement is induced by rainfall. The main hypothesis of the model is that the static friction decreases as a result of the rain, which acts as a lubricant and increases the mass of the units. Although the model is still schematic, missing known constitutive relations, its emerging behavior is quite promising.

2 The model and simulation methodology

We limit the study to two-dimensional simulations (seen from above) along a slope, modeling shallow landslides. We consider $N$ particles, initially arranged in a regular grid (Fig. 1), all of radius $r$ and mass $m$. 
The idea is to simulate the dynamics of these particles during and after a rainfall. In the model the rain has two effects: the first causes an increase in the mass of particles, while the second involves a reduction in static friction between the particle and the surface below.

The equation of Mohr-Coulomb,
\[ \tau_f = c' + \sigma' \tan(\phi'), \]

says that the shear stress \( \tau_f \) on the sliding surface is given by an adhesive part \( c' \) plus a frictional part \( \tan(\phi') \). In the our model we want to find a trigger condition of the particle that is based on the law of Mohr-Coulomb (Eq. (1)).

The coefficient of cohesion, \( c' \) in the Eq. (1), has been modeled by a random coefficient that depends on the position of the surface. On the other hand, the term \( \sigma' \tan(\phi') \) in the Eq. (1), has been modeled by a theoretical force of static friction \( F_i^{(s)} \) which is described later.

The static-dynamic transition is based on the following trigger conditions:
\[ |F_i^{(a)}| < F_i^{(s)} + c', \]
\[ |v_i| < v_i^{(threshold)} \to 0, \]  

then the motion of the single block will not be triggered until the active forces \( F_i^{(a)} \) (gravity forces + contact forces) do not exceed the static friction \( F_i^{(s)} \) plus the cohesion term \( c' \) and until the velocity \( |v_i| \) not overcomes the threshold velocity \( v_i^{(threshold)} \) (Eq. (2)). The irregularities of the surface are modeled by means of the friction coefficients, which depends stochastically on the position (quenched disorder).

In Eq. (2), the force \( F_i^{(a)} \) is given by the sum of two components: the gravity \( F_i^{(g)} \) and the interaction between the particles \( F_i^{(i)} \).
\[ F_i^{(a)} = F_i^{(g)} + F_i^{(i)}. \]  

The gravity \( F_i^{(g)} \) is given by
\[ F_i^{(g)} = g \sin(\alpha)(m_i + w_i(t)), \]
Fig. 2. (a) Particles in the computational domain: the maximum radius of iteration defined in the algorithm is equal to the side $L$ of the cell. Considering the black particle in the center of the circumference, it can interact only with the neighboring blue particles. (b) Cells considered when calculating the forces: if a particle is in cell $(x, y)$, the interaction forces will be calculated considering only the particles located in cells $(x + 1, y)$, $(x + 1, y + 1)$, $(x + 1, y)$ and $(x - 1, y)$. This method halves the number of interactions because it calculates 4 cells instead of 8.

where $g$ is the acceleration of gravity, $\alpha$ the slope (supposed constant) of the surface, $m_i$ the dry mass of block $i$ and $w_i$ the absorbed water cumulated in time. The quantity $w_i(t)$ is a stochastic variable (corresponding to rainfall events $\sigma^{(w)}(t)$),

$$w_i(t) = \int \sigma^{(w)}(t) \, dt.$$

The interaction force between two particles is defined through a potential that, in the absence of experimental data, we modeled after the Lennard-Jones one. The corresponding interaction force $F_{ij}^{(i)}$ that acts on block $i$ due to block $j$ is given by

$$F_{ij}^{(i)} = -F_{ji}^{(i)} = -\nabla V(R_{ij}) = -\nabla \left( 4\epsilon \cdot \left[ \left( \frac{r}{R_{ij}} \right)^{-12} - \left( \frac{r}{R_{ij}} \right)^{-6} \right] \right),$$

where $R_{ij}$ is the distance between the particles,

$$R_{ij} = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2},$$

$r$ is the radius of the particles and $\epsilon$ is a constant.

The computational strategy for calculating the interaction forces between the particles is similar to the Verlet neighbor list algorithm (art:verlet). In the code the computational domain is divided in square cells of side $L$ (see Fig. 2 (a)), corresponding to the length at which the interaction force is truncated. The truncation has a very little effect on the dynamics, so we did not correct the potential by setting $V(L) = 0$, as usual in MD.
Fig. 3. (a) Static friction coefficient $\mu_s$ vs. time, with $\mu_s^{(0)} = 1.2$ and $\mu_s^{(\infty)} = 0.4$. (b) Triggering time vs. slope, Eq. 18 with $m = 0.01$, $c' = 0.1$, $\mu_s^{(0)} = 1.15$ and $\mu_s^{(\infty)} = 0.45$.

Thanks to the Newton’s third law it is possible reduce the number interaction and consider the only particle that has not been considered in the previous step (see Fig. 2(b)).

The condition of motion for a given particle is governed by Eq. 2. The static friction $F_s^{(s)}$ is given by

$$F_s^{(s)} = \mu_s(m_i + w_i(t)) \cos(\alpha).$$

Eq. (8) is expressed by the friction’s coefficient $\mu_s$. We assumed that the rain has a lubricating effect between the particles and underlying surface; the friction coefficient has therefore been defined as,

$$\mu_s = \mu_s^{(\infty)} + (\mu_s^{(0)} - \mu_s^{(\infty)}) \exp(-w_0 t),$$

Eq. (9) where $\mu_s^{(0)}$ and $\mu_s^{(\infty)}$ are, respectively, the initial (dry) friction coefficient at $t = 0$ (starting of rainfall) and the final (wet) for $t \to \infty$. The effect of rainfall is to lubricate the sliding surface of the landslide, at a constant speed $w_0$ in this example.

When the active forces exceed the static friction plus the quenched stochastic coefficient of cohesion $c'$, the particle start to move. In this case the force acting on the particle $i$ is given by

$$F_i = F_i^{(a)} - F_i^{(d)},$$

where $F_i^{(a)}$ are the active forces, and $F_i^{(d)}$ is the force of dynamic friction,

$$F_i^{(d)} = \mu_d(m_i + w_i(t)) \cos(\alpha).$$

Eq. (11) is of the same type as Eq. (8); the coefficient of dynamic friction $\mu_d$ is defined similarly to the static one (Eq. (9)). The friction coefficients (static and dynamic) varies from point to point of the computational domain this choice serves to model the sliding surface like a rough surface.
When a particle exceed the threshold condition (Eq. 2), it moves on the slope with an acceleration \( a \) equal to

\[ a = \frac{F_i}{(m_i + w_i(t))}. \] (12)

In MD the most widely used algorithm for time integration is the Verlet algorithm. This algorithm allows a good numerical approximation and is very stable. It also does not require a large computational power because the forces are calculated once for each time step. The model was implemented using the second-order Verlet algorithm. We first compute the displacement of particles, and half of the velocity updates,

\[ r'_i = r_i + v_i \Delta t + \frac{F_i}{2m_i} \Delta t^2, \]

\[ v'_i = v_i + \frac{F_i}{2m_i} \Delta t, \] (13)

then compute the forces \( F'_i \) as function of the new positions \( r'_i \), and finally compute the second half of velocities,

\[ v''_i = v'_i + \frac{F'_i}{2m_i} \Delta t. \] (14)

We have to define a landslide-triggering time, for instance the time of the first moving block. In case of constant mass, it is very simple to obtain the trigger time theoretically. We can write, in equilibrium conditions, for a given mass

\[ |F_i| = F_i^{(s)} + c', \]

\[ F_i = F_i^{(g)} + F_i^{(s)} \] (15)

We assume that the first movement of the particle is only due to the effect of gravity, so that we can set the interaction forces equal to zero, and therefore the equilibrium condition is given by

\[ |F_i| = F_i^{(g)} + c', \] (16)

i.e.,

\[ \hat{m}g \sin(\alpha) = \hat{m} \cdot g \cos(\alpha) \{ \mu_s^{(0)} \exp(w_0 \cdot t) + \mu_s^{(\infty)}[1 - \exp(-w_0t)]\} + c', \] (17)

where \( \hat{m} = m + w(t) \), but Eq 17 is solvable analytically for \( \hat{m} = m + \delta \omega \) (\( \delta \omega \) is constant rain).

Therefore, using Eq 17 we can define the trigger time \( T \) in case of constant mass \( \hat{m} \) as:

\[ T = -\frac{1}{w_0} \cdot \log \left( \frac{\tan(\alpha) - \frac{c'}{\mu_s^{(0)} - \mu_s^{(\infty)}}}{\mu_s^{(0)} - \mu_s^{(\infty)}} \right). \] (18)
Table 1. Parameter values used in simulations

<table>
<thead>
<tr>
<th>Sim</th>
<th>m</th>
<th>r</th>
<th>cell</th>
<th>$\mu_s^{(0)}$</th>
<th>$\mu_s^{(\infty)}$</th>
<th>$\mu_d^{(0)}$</th>
<th>$\mu_d^{(\infty)}$</th>
<th>$c'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0001</td>
<td>0.5</td>
<td>1 x 1</td>
<td>1.15</td>
<td>0.7</td>
<td>0.65</td>
<td>0.34</td>
<td>0.01+\epsilon</td>
</tr>
<tr>
<td>1b</td>
<td>0.0001</td>
<td>0.5</td>
<td>1 x 1</td>
<td>1.15</td>
<td>0.7</td>
<td>0.65</td>
<td>0.34</td>
<td>0.01+\epsilon</td>
</tr>
<tr>
<td>2</td>
<td>0.0001</td>
<td>0.5</td>
<td>1 x 1</td>
<td>1.15</td>
<td>0.7</td>
<td>0.65</td>
<td>0.34</td>
<td>1+\epsilon</td>
</tr>
<tr>
<td>3</td>
<td>0.0001</td>
<td>0.5</td>
<td>1 x 1</td>
<td>0.85</td>
<td>0.4</td>
<td>0.35</td>
<td>0.14</td>
<td>0.01+\epsilon</td>
</tr>
</tbody>
</table>

3 Results

In order to simulate a landslide along an inclined plane, we use the theoretical model as described above with different parameters.

In the Table 1 we illustrate the parameters used in different simulations, where Sim is the number of simulation, $m$ and $r$ are respectively the mass and the radius of the particles, $\mu_s^{(0)}$, $\mu_s^{(\infty)}$, $\mu_d^{(0)}$, $\mu_d^{(\infty)}$ are the coefficients of static and dynamic friction and $c'$ is the coefficient of cohesion. In our simulations the time $dt$ of simulation is set to 0.01: then the effective time $t$ is different from the simulation time $T$.

3.1 Simulation 1

The position of the particles at $t = 3000$ is reported in Fig. 4. The rain starts with the particles at rest. We suppose that the speed of the landslide is much bigger than the rain flux, so that the computation of sliding is performed without the contribution of rain (i.e., instantaneously). The rain increases the mass of the particle with a factor between 0 and 0.0001. The graph of the kinetic energy (Fig. 5) shows a "stick-slip" dynamic. The distribution $f(x)$ the kinetic energy (Fig. 6) is well approximated by an exponential

$$f(x) = a \cdot e^{bx}, \tag{19}$$

with $a \simeq 3.2 \cdot 10^4$ and $b \simeq -0.1042$.

In Fig. 7 the statistical distribution of the intervals between trigger times is reported. This distribution is well fitted by a power law

$$f(x) = a \cdot x^b, \tag{20}$$

with $a \simeq 691.1$ and $b \simeq -0.4295$.

Several authors have observed that some natural hazards such as landslides, earthquakes and forest fires exhibit a power law distribution [10–12].

3.2 Simulation 1b

In this simulation we use the same parameters as in simulation 1, but we stop the rain event at time $t = 20$. This is a special case: we want to study the effect of a steady rain until a fixed time. Fig. 8 shows the arrangement of the particles and Fig. 9 the kinetic energy at $t = 300$.

One can note that the maximum kinetic energy is much greater in this simulation. In the case 1 the maximum value of kinetic energy is $5.74 \cdot 10^{-4}$ while here it is $2.6 \cdot 10^{-3}$. Many small events are observed in the first case while in the present one we observe a single large event.
Fig. 4. (a) Position of particles in Simulation 1 at $t = 3000$.

Fig. 5. (b) Kinetic energy vs. time.

Fig. 6. (a) Frequency distribution of the kinetic energy in Simulation 1. The plot in semi-log axes shows an exponential distribution.

Fig. 7. (b) Frequency distribution of trigger intervals in Simulation 1. The plot in log-log axes shows a power-law distribution.

3.3 Simulation 2

In order to explore the dependence of the system behavior on the coefficient of cohesion $c'$, we vary it from 0.01 to 1. The other parameters are the same of Simulation 1. We observe that the final disposition of the particles (Fig. 10) is not too different from Simulation 1 (Fig. 4), however, it occurs at time $t = 7500$ versus $t = 3000$ of Simulation 1.

As reported in Fig. 11, the increase of the cohesion coefficient $c'$ causes a time dilatation, i.e., a translation of the time at which similar events occur.

3.4 Simulation 3

We explore here the behavior of the system as a function of coefficients of static and dynamic friction $\mu_s$ and $\mu_d$. Their values are shown in Table 1. The other parameters are the same of Simulation 1. The consequence of the reduction of friction causes an immediate movement of particles. Moreover the number of particles involved during the event are larger then in the previous simulations (Fig. 13).
Fig. 8. (a) Position of particles in Simulation 1b at $t = 300$.
Fig. 9. (a) Kinetic energy versus time. We observe that the "stick-slip" events disappear and the fixed duration of precipitation changes the dynamics of the system: in particular, there is a peak at $t = 20$ at the end of the rain event.

Fig. 10. (a) Position of particles in Simulation 2 at $t = 7000$. We observe that to have a spatial arrangement of particles similar to those of the previous simulation (Fig. 4) a larger time is needed.
Fig. 11. (b) Kinetic energy of the systems versus time. The black line is the kinetic energy of Simulation 2. Comparing it with Fig. 5 of Simulation 1, we observe that an increase in the cohesion coefficient induces a translation of the events.

Fig. 16 shows that also in this case the statistical distribution of the kinetic energy follows an exponential distribution. The data fit of Eq. (19) gives $a \approx 2.592 \cdot 10^4$ and $b \approx -0.091$.

4 Conclusions

In this article we presented a theoretical model that may be useful for studying the effect of precipitation on granular materials. The main hypothesis is that the rain acts as a lubricant between the terrain and the granular: this effect has been modeled by a preliminary report that includes the reduction of static (or dynamic) friction when we simulate the rainfall (Eq. (8) and Eq. (11)). The reduction in friction allows to follow the evolution and change in the position of the particles during and after a rainfall. The results obtained are very encouraging as regards both the displacement and evolution of the particles and
Fig. 12. (a) Position of particles in Simulation 3 at $t = 3000$. The gray area represents the particle position of Simulation 1 (Fig. 4).

Fig. 13. (b) Number of particles involved. The decrease of the friction coefficients leads to an increase in the number of particles in motion.

Fig. 14. (a) Kinetic energy of the systems vs. time. The black line is the kinetic energy of Simulation 3. In the last simulation the value of the kinetic energy is greater than that in Simulation 1. This is due by the number of particles involved in the event (Fig. 13).

Fig. 15. (b) Mean velocity of the system versus time after $t = 1000$ for Simulations 1 and 3. We can observe that the two values are not too different between the two simulations. The difference of the kinetic energy is due to the number of particle in movement.

In the statistical properties of the system. The next step will be to develop an experimental setup where granular material (sand or gravel) will be placed on a sloping surface: through liquid lubricant (soap and water) we will study the dynamics of these particles. The comparison of experimental and computational model will be very useful for the analysis of the effect of lubrication of the soil caused by rainfall.
157

Fig. 16. (a) Statistical distribution of kinetic energy in Simulation 3. It follows an exponential distribution like in Simulation 1.

Fig. 17. (b) The blue line refers to Simulation 3 with parameters $a_3 \approx 2.88 \cdot 10^5$ and $b_3 \approx -2.365$. The black line refers to Simulation 1 with parameters $a_1 \approx 2.83 \cdot 10^5$ and $b_1 \approx -3.078$. The dots represent the normalized value of the respective simulations.

References

Projective synchronization of different chaotic
discrete-time neural networks with delays, based on
impulsive controllers

Eva Kaslik\textsuperscript{1,2} and Seenith Sivasundaram\textsuperscript{3}

\textsuperscript{1} Institute e-Austria Timisoara, Romania
\textsuperscript{2} Department of Mathematics and Computer Science
west University of Timisoara, Romania
\textsuperscript{3} Department of Mathematics
Embry-Riddle Aeronautical University, Daytona Beach, FL 32114, USA

\textbf{Abstract.} In this paper, an impulsive control approach is presented for the projective synchro-

nization of two different chaotic Hopfield-type discrete-time neural networks with delays. The
global asymptotic stability of the error dynamical system is studied, using linear matrix in-

equalities, vector Lyapunov functions and the stability theory of impulsive systems. Simulation
eXamples are given to illustrate the feasibility and effectiveness of the proposed approach.

\textbf{Keywords:} projective synchronization, impulsive control, neural network.

\section{Introduction}

In recent years, we have seen a rapid growth of theoretical and experimental studies on
chaos synchronization due to potential applications in secure communication, inform-

ation processing, pattern formation, etc. One of the chaos synchronization methods
that is most often discussed is the master-slave scheme, introduced by Pecora and Carroll \cite{1,2}.

Impulsive synchronization allows the synchronization of the master and slave sys-
tems using small impulses generated by samples (called synchronizing impulses) of
the state variables of the master system, only at discrete time instances. This dra-

stically reduces the amount of information transmitted from the master system to the
slave system, making this method more efficient and useful in a great number of real-
life applications. After a finite period of time, the two systems behave in accordance
with each other and synchronization is achieved. In other words, this is equivalent
to the attractivity of the null solution of the error dynamics between the master and
slave systems. Therefore, the qualitative theory of impulsive dynamical systems and
impulsive control \cite{3–5} plays a fundamental role in impulsive synchronization.

Impulsive synchronization has been applied to a number of chaos-based secure
communication systems, exhibiting good performance and proving to be more robust
than continuous synchronization [6–9]. Recently, a large number of papers discussed impulsive synchronization in continuous-time neural networks [10–15] and dynamical networks [16–21], but very few refer to discrete-time networks [22–24].

Another interesting research problem is projective synchronization, characterized by a scaling factor with respect to which two systems synchronize proportionally. Applied to secure communication, this feature can be used to M-nary digital communication for achieving fast communication. Projective synchronization phenomena were first reported by Gonzalez-Miranda [25] and Mainieri and Rehacek [26], who observed that when chaotic systems exhibit invariance properties under a special type of continuous transformation, amplification and displacement of the attractor occurs. Recently, several projective synchronization results have been presented for neural networks using the adaptive approach [27], integral sliding mode controllers [28], impulsive controllers [29] and the observer-based approach [30].

In this paper, projective synchronization results based on impulsive controllers are developed for two different chaotic Hopfield-type discrete-time neural networks with delays. The main synchronization result obtained here are based on linear matrix inequalities and the vector Lyapunov function method [31]. An illustrative example is also given, along with computer simulation results, with the aim of visualizing the satisfactory control performance.

2 Main results

In the following, we denote $\mathbb{Z}_{-\tau} = \{-\tau + 1, -\tau + 2, \ldots, 0\}$, $\mathbb{Z}^+ = \{1, 2, 3, \ldots\}$ and $\mathbb{Z}^+_0 = \{0, 1, 2, \ldots\}$.

Consider the general discrete-time delayed Hopfield-type neural network in the following matrix form:

\[
\begin{align*}
\begin{cases}
x(t) &= Ax(t - 1) + Tg(x(t - \tau)), \quad t \in \mathbb{Z}^+ \\
x(s) &= \phi_1(s), \quad s \in \mathbb{Z}_{-\tau}
\end{cases}
\end{align*}
\]

where the matrix $A$ is a diagonal matrix, the activation function $g$ is of the form $g(x) = (g_1(x_1), g_2(x_2), \ldots, g_n(x_n))^T$, $g(0) = 0$, $T = (T_{ij})_{n \times n}$ is the interconnection matrix and $\phi_1(s), s \in \mathbb{Z}_{-\tau}$ represent the initial conditions. For simplicity, we choose equal time delays, $\tau \in \mathbb{Z}^+$.

Consider that system (1) is the master system, while the slave system is:

\[
\begin{align*}
\begin{cases}
y(t) &= A'y(t - 1) + T'g'(y(t - \tau)), \quad t \in \mathbb{Z}^+ \\
y(t_k^+) &= y(t_k) + J_k(x, y), \quad k \in \mathbb{Z}^+ \\
y(s) &= \phi_2(s), \quad s \in \mathbb{Z}_{-\tau}
\end{cases}
\end{align*}
\]

where $A'$ is a diagonal matrix, $T' = (T'_{ij})_{n \times n}$ is the interconnection matrix, the function $g'$ is of the form $g'(x) = (g'_1(x_1), g'_2(x_2), \ldots, g'_n(x_n))^T$, $g'(0) = 0$, $J_k$ is the jump operator, $\phi_2(s), s \in \mathbb{Z}_{-\tau}$ represent the initial conditions, and the impulse times
In the slave system (2), the meaning of $y(t_k^+)\) is the following: $y(t_k^+)$ is computed from the first equation and then replaced by $y(t_k^-)$ according to the second equation (impulse effect).

Projective synchronization is achieved between the master and slave systems (1) and (2) if and only if

$$\lim_{t \to \infty} \|\rho x(t) - y(t)\| = 0 \quad (3)$$

where $\rho \in \mathbb{R}^*$ is the scaling factor which characterizes the projective synchronization.

In what follows, we will consider that the jump operator $J_k$ takes the form

$$J_k(x, y) = A_k(\rho x(t_{k-1}) - y(t_{k-1}))$$

where $A_k \in \mathbb{R}^{n \times n}$.

Let $e = \rho x - y$ be the error of the systems (1) and (2). It satisfies:

$$\begin{cases} 
    e(t) = Ae(t - 1) + (A - A')y(t - 1) + \\
    \quad + \Phi_\rho(x(t - \tau), y(t - \tau)), & t \in \mathbb{Z}^+ \\
    e(t_k^+) = (I - A_k)e(t_{k-1}), & k \in \mathbb{Z}^+ \\
    e(s) = \rho \phi_1(s) - \phi_2(s) = \phi_\rho(s), & s \in \mathbb{Z} - \tau 
\end{cases} \quad (4)$$

where $\Phi_\rho : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ is defined by

$$\Phi_\rho(x, y) = \rho T g(x) - T' g'(y).$$

In the following, consider $h_i : \mathbb{R}^2 \to \mathbb{R}$ defined by:

$$h_i(x, y) = \begin{cases} 
    \frac{g_i(x_i) - g_i(y_i)}{x_i - y_i} & \text{if } x_i \neq y_i \\
    \frac{0}{0} & \text{if } x_i = y_i 
\end{cases}$$

Let be the matrix function $H : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^{n \times n}$ by

$$H(x, y) = \text{diag}(h_1(x_1, y_1), h_2(x_2, y_2), ..., h_n(x_n, y_n)).$$

Since $g(x) = (g_1(x_1), g_2(x_2), ..., g_n(x_n))^T$, it follows that

$$g(x) - g(y) = H(x, y)(x - y).$$

On the other hand, let $k_i : \mathbb{R}^2 \to \mathbb{R}$ be defined by:

$$k_i(y_i) = \begin{cases} 
    \frac{g_i(y_i)}{y_i} & \text{if } y_i \neq 0 \\
    \frac{0}{0} & \text{if } y_i = 0 
\end{cases}$$
Considering the matrix function $K : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}$ given by

$$K(y) = \text{diag}(k_1(y_1), k_2(y_2), ..., k_n(y_n)),$$

it follows that

$$g(y) = K(y)y.$$

In the same way, we can express:

$$g'(y) = K'(y)y.$$

Therefore we obtain

$$\Psi \Phi \rho \in \Omega $$$$

The following theorem represents the main impulsive projective synchronization result for discrete-time delayed Hopfield neural networks.

**Theorem 1.** Let be a positive-definite matrix $P$, the dot product $\langle x, y \rangle = x^T Py$ and the corresponding vector norm $\| x \| = \sqrt{x^T P x}$. Assume that:

(i) There exist positive constants $\alpha_1, \alpha_2$ such that the matrix

$$M(x, y) = \begin{bmatrix}
    APA - \alpha_1 P & APA & APA(A - A') & APA \\
    \Psi^T PA & \Psi^T P \Phi - \alpha_2 P & \Psi^T P(A - A') & \Psi^T P \Omega \\
    (A - A')PA & (A - A')P \Phi & (A - A')P(A - A') & (A - A')P \Omega \\
    \Omega^T PA & \Omega^T P \Phi & \Omega^T P(A - A') & \Omega^T P \Omega
\end{bmatrix}$$


is negative semi-definite, for any \( x, y \in \mathbb{R}^n \). 

(ii) For any \( k \in \mathbb{Z}^+ \), there exist positive constants \( \beta_k \) such that the matrix

\[
M(k) = (I - A_k)^T P(I - A_k) - \beta_k P
\]

is negative semi-definite.

(iii) There exists \( c = [c_1, c_2, \ldots, c_\tau] \in (0, \infty)^\tau \) such that, defining the matrices \( Q_k \in \mathbb{R}^{\tau \times \tau} \) as

\[
Q_k = Q(\beta_k \alpha_1; \beta_k \alpha_2; c)Q(\alpha_1; \alpha_2; c)^{t_k - t_{k-1} - 1}
\]

with \( Q(u; v; c) \) given by (6), \( \alpha_1, \alpha_2 \), and \( \beta_k \) given by (i) and (ii), the following holds:

\[
\lim_{k \to \infty} \left( \prod_{i=1}^{k} Q_i \right) c = 0.
\]

Then the null solution of system (4) is globally attractive, i.e. the master system (1) and the slave system (2) are globally synchronized with scaling factor \( \rho \).

\textbf{Proof.} Let \( e(t) = e(t; t_0, \phi) \) be the solution of (4) with the initial condition \( \phi_{\rho}(s) \), \( s \in \mathbb{Z}_{-T} \). Consider the functional \( u(t) = ||e(t)||^2 = e(t)^T Pe(t) \).

Using \( \Psi \) and \( \Omega \) to denote \( \Psi(x(t-\tau), y(t-\tau)) \) and \( \Omega(x(t-\tau), y(t-\tau)) \), and \( B = A - A' \), from (i) we obtain:

\[
u(t) = \begin{bmatrix}
e(t-1) \\
e(t-\tau) \\
y(t-1) \\
y(t-\tau)
\end{bmatrix} = \begin{bmatrix}
\alpha_1 P & 0 & 0 & 0 \\
0 & \alpha_2 P & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
e(t-1) \\
e(t-\tau) \\
y(t-1) \\
y(t-\tau)
\end{bmatrix}
\]

\[
u(t) = \alpha_1 e(t-1)^T Pe(t-1) + \alpha_2 e(t-\tau)^T Pe(t-\tau) = \alpha_1 u(t-1) + \alpha_2 u(t-\tau)
\]

Moreover, using (ii) we have:

\[
u(t_k^+) = ||e(t_k^+)||^2 = ||(I - A_k)e(t_k)||^2 = e(t_k)^T (I - A_k)^T P(I - A_k)e(t_k)
\leq \beta_k e(t_k)^T Pe(t_k) = \beta_k u(t_k)
\]

Hence, \( u(t) \) satisfies the following inequalities:

\[
\begin{cases}
  u(t) \leq \alpha_1 u(t-1) + \alpha_2 u(t-\tau), & t \in \mathbb{Z}^+ \\
u(t_k^+) \leq \beta_k u(t_k), & k \in \mathbb{Z}^+
\end{cases}
\]  

(11)

In the rest of the proof, we will rely on the fact that if \( Q \) is a matrix with positive elements, the linear mapping \( w \mapsto Qw \) is non-decreasing, i.e. for any two vectors.
$w_1$, $w_2$ satisfying $w_1 \leq w_2$ we have $Qw_1 \leq Qw_2$ (the vector inequalities are considered component-wise).

We define the vector Lyapunov function $V : \mathbb{Z}_0^+ \rightarrow \mathbb{R}^r$

$$V(t) = [c_1u(t) \ c_2u(t-1) \ ... \ c_\tau u(t-\tau + 1)]^T \quad (12)$$

From the first inequality from (11) it is easy to see that

$$V(t) \leq Q(\alpha_1; \alpha_2; c)V(t-1), \forall t \in \mathbb{Z}^+$$

Hence:

$$V(t) \leq Q(\alpha_1; \alpha_2; c)\mathbf{u}(t_k), \forall t \in (t_k, t_{k+1}] \cap \mathbb{Z} \quad (13)$$

The two inequalities from (11) imply

$$u(t_k^+) \leq \beta_k \alpha_1 u(t_k - 1) + \beta_k \alpha_2 u(t_k - \tau)$$

which leads to

$$V(t_k^+) \leq Q(\beta_k \alpha_1; \beta_k \alpha_2; c)\mathbf{V}(t_k - 1), \forall k \in \mathbb{Z}^+$$

From (13) we obtain

$$V(t_k^+) \leq Q(\beta_k \alpha_1; \beta_k \alpha_2; c)Q(\alpha_1; \alpha_2; c)^{t_k - t_{k-1}}V(t_{k-1}^+) = Q_k V(t_{k-1}^+), \forall k \in \mathbb{Z}^+$$

and hence

$$V(t_k^+) \leq \prod_{i=1}^{k} Q_i V(0), \forall k \in \mathbb{Z}^+ \quad (14)$$

We have

$$V(0) = [c_1u(0) \ c_2u(-1) \ ... \ c_\tau u(-\tau + 1)]^T \leq \max_{s \in \mathbb{Z}_{-\tau}} u(s) \ c = \max_{s \in \mathbb{Z}_{-\tau}} \|\mathbf{e}(s)\|^2 \ c = \max_{s \in \mathbb{Z}_{-\tau}} \|\phi_p(s)\|^2 \ c$$

From inequality (14) we obtain

$$V(t_k^+) \leq \max_{s \in \mathbb{Z}_{-\tau}} \|\phi_p(s)\|^2 \left(\prod_{i=1}^{k} Q_i\right) \ c$$

Taking into account (iii), we obtain

$$\lim_{k \rightarrow \infty} V(t_k^+) = 0$$

From (13) we have

$$\|V(t)\|_\tau \leq \|Q(\alpha_1; \alpha_2; c)^{t-t_k} V(t_k^+)\|_\tau \leq \|Q(\alpha_1; \alpha_2; c)^{t-t_k} \|_\tau \|V(t_k^+)\|_\tau \leq \|Q(\alpha_1; \alpha_2; c)\|_\tau \|V(t_k^+)\|_\tau \leq \|Q(\alpha_1; \alpha_2; c)\|_\tau \|V(t_k^+)\|_\tau, \forall t \in (t_k, t_{k+1}] \cap \mathbb{Z}$$
which implies that \( \lim_{t \to \infty} V(t) = 0 \). As

\[
\|e(t)\|^2 = u(t) \leq \frac{1}{c_1} \|V(t)\|_r
\]

it follows that \( e(t) \) tends to 0 as \( t \) tends to infinity, which completes the proof. \( \Box \)

The Schur complement [32] is a useful tool for establishing whether a matrix is positive (or negative) (semi-)definite. We have the following result.

**Proposition 1 (See [32].)** Let \( M \in \mathbb{R}^{n \times n} \) be a symmetric matrix partitioned as

\[
M = \begin{bmatrix}
M_{11} & M_{12} \\
M_{12}^T & M_{22}
\end{bmatrix}
\]

in which \( M_{11} \) is square and nonsingular. Let \( M/M_{11} = M_{22} - M_{12}M_{11}^{-1}M_{12} \) denote the Schur complement of \( M_{11} \). Then:

(a) \( M > 0 \) if and only if \( M_{11} > 0 \) and \( M/M_{11} > 0 \);

(b) \( M \geq 0 \) if and only if \( M_{11} > 0 \) and \( M/M_{11} \geq 0 \).

where \( " > 0" \) means positive definite and \( " \geq 0" \) means positive semi-definite.

**Remark 1.**

(i) If \( T'g'(y) = \rho Tg(\rho^{-1}y) \), it follows that \( \Omegag(\rho) = 0 \). Moreover, if \( A = A' \), we can easily see that the matrix \( M(x, y) \) given by (7) becomes:

\[
M(x, y) = \begin{bmatrix}
APA - \alpha_1 P & AP\Psi \\
\Psi^T PA & \Psi^T P\Psi - \alpha_2 P
\end{bmatrix}
\]

Therefore, the Schur complement \( M/M_{11} = 0 \), and the matrix \( M(x, y) \) is negative semi-definite if and only if

\[
M_{11}(x, y) = \begin{bmatrix}
APA - \alpha_1 P & AP\Psi \\
\Psi^T PA & \Psi^T P\Psi - \alpha_2 P
\end{bmatrix} < 0
\]

(ii) More, if \( A = aI \), with \( a \in (0, 1) \), the matrix \( M_{11}(x, y) \) given above becomes:

\[
M_{11}(x, y) = \begin{bmatrix}
(a^2 - \alpha_1)P & aP\Psi(x, y) \\
\alpha\Psi(x, y)^T P \Psi(x, y) - \alpha_2 P
\end{bmatrix}
\]

Since \( P > 0 \), we have that \( (M_{11})_{11} = (a^2 - \alpha_1)P < 0 \) if and only if \( \alpha_1 > a^2 \).

The Schur complement of \( (M_{11})_{11} \) is

\[
M_{11}/(M_{11})_{11} = \frac{\alpha_1}{\alpha_1 - a^2} \Psi(x, y)^T P\Psi(x, y) - \alpha_2 P
\]

and taking into account that \( \Psi(x, y) = TH(x, y) \) we obtain

\[
M_{11}/(M_{11})_{11} = \frac{\alpha_1}{\alpha_1 - a^2} H(x, y)TPTH(x, y) - \alpha_2 P
\]
Assuming that the activation functions $g_i$ are Lipschitz continuous, it follows that there exists $L > 0$ such that $|h_i(x, y)| \leq L$ for any $i = 1, n$. Therefore, we obtain that

$$M_{11}/(M_{11})_{11} \leq \frac{\alpha_1 L^2}{\alpha_1 - a^2} T^T P T - \alpha_2 P$$

If the right hand side of this inequality is negative definite, it follows that $M_{11}/(M_{11})_{11}$ is negative definite as well.

**Remark 2.** If $A_k = a_k I, a_k \in \mathbb{R}$, the matrix $M(k)$ given by (8) becomes:

$$M(k) = [(1 - a_k)^2 - \beta_k]P$$

and it is negative semi-definite if and only if $(1 - a_k)^2 \leq \beta_k$.

**Remark 3.** Condition (iii) of Theorem 1 means that the solution of the linear system

$$z_{k+1} = Q_k z_k \quad \text{(in } \mathbb{R}^T \text{)}$$  \hspace{1cm} (15)

with the initial condition $z_0 = c$, converges to 0.

If for any $k \in \mathbb{Z}$ we have $\beta_k = \beta$, the matrices $Q_k$ defined by (9) become:

$$Q_k = Q(\beta \alpha_1; \beta \alpha_2; c)Q(\alpha_1; \alpha_2; c)^{t_k - t_{k-1} - 1}$$

Since $\delta \leq t_k - t_{k-1} \leq \Delta$, it follows that for any $k \in \mathbb{Z}$, the matrix $Q_k$ belongs to the finite set of matrices

$$Q = \{Q(\beta \alpha_1; \beta \alpha_2; c)Q(\alpha_1; \alpha_2; c)^{m-1}, m \in \{\delta, \delta + 1, ..., \Delta\}\}.$$  

Therefore, the system (15) is a switching system.

Moreover, if $t_k - t_{k-1} = \delta = \Delta$ for any $k \in \mathbb{Z}$, then the system (15) reduces to an autonomous linear system, with the matrix $Q = Q(\beta \alpha_1; \beta \alpha_2; c)Q(\alpha_1; \alpha_2; c)^{\Delta-1}$. In this case, condition (iii) of Theorem 1 is equivalent to $c$ belonging to the stable eigenspace of the matrix $Q$.

In the following, based on the results obtained in Theorem 1, sufficient conditions for the impulsive projective synchronization of non-delayed neural networks will be given. With this aim, we will consider $\tau = 1$ in systems (1), (2) and (4).

**Proposition 2.** Assume that $\tau = 1$. Let be a positive-definite matrix $P$, the dot product $\langle x, y \rangle = x^T P y$ and the corresponding vector norm $\|x\| = \sqrt{x^T P x}$. Assume that:

(i) there exist positive constants $\alpha_1, \alpha_2$ and $\beta_k$ such that conditions (i) and (ii) of Theorem 1 holds.

(ii) there exists $\epsilon \in (0, 1)$ such that

$$\beta_k (\alpha_1 + \alpha_2)^{t_k - t_{k-1}} \leq \epsilon, \forall k \geq \tilde{k}.$$  

Then the null solution of system (4) is globally attractive, i.e. the master system (1) and the slave system (2) are globally synchronized with scaling factor $\rho$. 

The trajectory of (16) is shown in Fig. 2. 

We consider the following master system 

\begin{align*}
Q_k &= \beta_k (\alpha_1 + \alpha_2)^{t_k - t_{k-1}} \leq \epsilon, \quad \forall k \geq \tilde{k}.
\end{align*}

Hence for any $k \geq \tilde{k}$ we have

\begin{align*}
\prod_{i=1}^{k} Q_i \leq \epsilon^{k-\tilde{k}} \prod_{i=1}^{\tilde{k}} Q_i \xrightarrow{k \to \infty} 0
\end{align*}

and based on Theorem 1, the proof is complete. □

3 Example

We consider the following master system

\begin{align*}
\begin{cases}
x_1(t) = a x_1(t-1) + T \tanh(x_3(t-\tau)) \\
x_2(t) = a x_2(t-1) + T \sin(x_3(t-\tau)) \\
x_3(t) = a x_3(t-1) + T \tanh(x_2(t-\tau))
\end{cases}, \quad t \in \mathbb{Z}^+ \quad (16)
\end{align*}

where $a = 0.5$ and $\tau = 3$.

Based on the theoretical results obtained in [33], it can be shown that the null solution of (16) is asymptotically stable if and only if $T \in (-0.534, 0.5)$. At $T = 0.5$ a Cusp bifurcation takes place in system (16) and at $T = -0.534$ a supercritical Neimark-Sacker bifurcation occurs. If $|T|$ is sufficiently large, the system (16) will exhibit chaotic behavior.

The Lyapunov characteristic exponents for $T \in (-2, 0)$ are presented in Fig. 1. The collision of the two largest Lyapunov exponents for $T = -0.534$ corresponds to the supercritical Neimark-Sacker bifurcation. For $T \in (-1.52, -0.534)$, the largest Lyapunov exponent is null, which corresponds to the existence of an asymptotically stable limit cycle. As $T$ decreases below $-1.52$, the largest Lyapunov exponent becomes positive, suggesting chaotic behavior in system (16).

For example, for $T = -1.7$ we obtain that the two largest Lyapunov exponents are positive: 0.03 and 0.002 respectively. Hence, the system (16) is hyperchaotic in a neighborhood of the null solution. Indeed, considering the initial conditions:

\begin{align*}
x(-2) &= (-2.86584, 0.438859, 1.73719) \\
x(-1) &= (-3.12197, 1.91191, 0.620975) \quad (17) \\
x(0) &= (-3.24297, 2.1437, 1.88233)
\end{align*}

the trajectory of (16) is shown in Fig. 2.

The slave system that we consider for projective synchronization is

\begin{align*}
\begin{cases}
y_1(t) = a y_1(t-1) + T \rho \tanh(\rho^{-1} y_3(t-\tau)) \\
y_2(t) = a y_2(t-1) + T \rho \sin(\rho^{-1} y_1(t-\tau)) \\
y_3(t) = a y_3(t-1) + T \rho \tanh(\rho^{-1} y_2(t-\tau)) \\
y(t_k) = y(t_k) + a_k (\rho x(t_k) - y(t_k)) \quad , \quad k \in \mathbb{Z}^+
\end{cases}
\end{align*}

with $\rho = 0.5$, $a_k = 0.7$ and $t_k = 8k$.

Null initial conditions have been considered for the slave system. Figures 3-5 show that projective synchronization is achieved with scaling factor $\rho = 0.5$. 

Proof. To verify that condition (iii) of Theorem 1 is also fulfilled, it is enough to notice that since $\tau = 1$, we have:

\begin{align*}
Q_k &= \beta_k (\alpha_1 + \alpha_2)^{t_k - t_{k-1}} \leq \epsilon, \quad \forall k \geq \tilde{k}.
\end{align*}

The Lyapunov characteristic exponents for (16) are presented in Fig. 1. At $T = 0.5$ a Cusp bifurcation takes place in system (16) and at $T = -0.534$ a supercritical Neimark-Sacker bifurcation occurs. If $|T|$ is sufficiently large, the system (16) will exhibit chaotic behavior.

Based on the theoretical results obtained in [33], it can be shown that the null solution of (16) is asymptotically stable if and only if $T \in (-0.534, 0.5)$. At $T = 0.5$ a Cusp bifurcation takes place in system (16) and at $T = -0.534$ a supercritical Neimark-Sacker bifurcation occurs. If $|T|$ is sufficiently large, the system (16) will exhibit chaotic behavior.
Fig. 1. Lyapunov characteristic exponents for $T \in (-2, 0)$.

Fig. 2. Trajectory of the master system (16) with $T = -1.7$ and initial conditions (17) (5000 iterations have been plotted).

Fig. 3. Trajectory of the slave system (18) with $T = -1.7$ and null initial conditions (5000 iterations have been plotted).
Fig. 4. Norm of the synchronization error $e(t) = \rho x(t) - y(t)$.

Fig. 5. Evolution of $x_i$ (blue - master system) versus $y_i$ (red - slave system), $i = 1, 2, 3$.

4 Conclusions

In this paper, sufficient conditions for the projective synchronization by impulsive controllers of general delayed discrete-time neural networks have been given. Numerical results show good agreement with the theoretical findings. Extending these results to more complicated neural network models with different types of time-delays may constitute a direction for future research.
Acknowledgements

This work was supported by CNCSIS-UEFISCSU, project number PN-II-RU-PD-145/2010 (Advanced impulsive and fractional-order neural network models).

References

Simulations of the Frequency Modulated - Atomic Force Microscope (FM-AFM) Nonlinear Control System

Átila M. Bueno¹, José M. Balthazar¹, and José R. C. Piqueira²

¹ Universidade Estadual Paulista UNESP, Departamento de Estatística Matemática Aplicada e Computação DEMAC/IGCE, Rio Claro, SP, CP 178, CEP 13506-900, Brazil
(E-mail: atila@lac.usp.br, jmbaltha@rc.unesp.br)
² Escola Politécnica, Universidade de São Paulo, Av. Prof. Luciano Gualberto, travessa 3, n. 158, 05508-900, São Paulo, SP, Brazil
(E-mail: piqueira@lac.usp.br)

Abstract. The Frequency Modulated - Atomic Force Microscope (FM-AFM) is a powerful tool to perform surface investigation with true atomic resolution. The control system of the FM-AFM must keep constant both the frequency and amplitude of oscillation of the microcantilever during the scanning process of the sample. However, tip and sample interaction forces cause modulations in the microcantilever motion. A Phase-Locked Loop (PLL) is used as a demodulator and to generate feedback signal to the FM-AFM control system. The PLL performance is vital to the FM-AFM performance since the image information is in the modulated microcantilever motion. Nevertheless, little attention is drawn to PLL performance in the FM-AFM literature. Here, the FM-AFM control system is simulated, comparing the performance for different PLL designs.

Keywords: Frequency Modulated Atomic Force Microscope, Phase-Locked Loops, Synchronization.

1 Introduction

The Atomic Force Microscopy started with the development of the Atomic Force Microscope (AFM) in 1986 by G. Binnig [1]. Simple contact measurement techniques resulted in many discoveries and developments to the surface investigation science. However, contact AFM cannot generate true atomic resolution images in a stable operation, and the samples are frequently damaged due to the contact with the microcantilever tip during the scanning process. On the other hand, noncontact AFM achieve true atomic resolution without damaging the samples.

The Frequency-Modulated Atomic Force Microscope (FM-AFM) is a noncontact AFM technique. In the FM-AFM the microcantilever is deliberately
vibrated (Fig. 1) and is driven to oscillate at a fixed amplitude and frequency [2,3] by the Automatic Gain Control loop (AGC) and by the Automatic Distance Control (ADC) loop, respectively. In addition, the AGC and ADC control systems generate the dissipation and topographic images (Fig. 2).

In the FM-AFM the feedback signal is provided by the Phase-Locked Loop (PLL) present in the FM-AFM control system [4-6] demodulating the tip and sample interaction forces used by the ADC. The PLL also synthesizes the AGC signal (Fig. 2) in order to control the microcantilever oscillation amplitude.

The PLL (Fig. 3) is a control system that synchronizes a local oscillator to an incoming signal, playing important roles in communication, computation.

---

**Fig. 1.** Schematic view of the microcantilever oscillation

**Fig. 2.** FM-AFM control system
and control systems [7,8]. PLLs are nonlinear devices and behaviors such as bifurcations and chaos may arise [9,11]. Additionally, ripple oscillations such as the Double Frequency Jitter (DFJ), generated by the Phase Detector (PD), corrupts the synchronization quality [12]. Therefore, PLL design is crucial to demodulation systems and consequently to FM-AFM.

Fig. 3. PLL block diagram

In section 2 the FM-AFM mathematical model is presented. In section 3 the lock-in range of the third order PLL with second order Salley-Key filter is determined by means of bifurcation analysis. In addition a design technique is discussed. In section 4 the simulations results are shown.

2 FM-AFM Mathematical Model

The mathematical model for the FM-AFM is obtained, considering the external driving signal and the tip-sample interaction, the amplitude detector and the PLL. The modeling follows what was presented in [4].

2.1 The Micro-Cantilever

The micro-cantilever is considered to be a damped second order system that can be described by the equation:

\[
\ddot{z}(t) + \gamma \dot{z}(t) + \omega_n^2 z(t) = r(t)v(t) + F_{ts}(z, d)
\]  

(1)

where \(z(t)\) is the micro-cantilever tip position, \(\gamma\) is the damping factor, \(\omega_n\) is the natural frequency of the micro-cantilever and \(d\) is the tip height (see Fig. 1). \(F_{ts}(z, d)\) is the tip and sample interaction force, \(r(t)\) controls the amplitude of the oscillation and \(v(t)\) is the PLL output signal [2,3,5,6].

The FM-AFM operates in a long range distance between tip and sample, and considering that the tip and sample are not conductive, \(F_{ts}\) is mainly due to the van der Waals force, given by:

---

The photodiode response is considered to be fast, and therefore it is neglected.
where $A_H$ is the Hamaker constant that depends on the type of materials of the tip and sample [3]. It can be seen in Fig. 2 that $r(t)$ is the control signal from the AGC. However, the tip and sample interaction force $F_{ts}(z, d)$ generates modulations on both the amplitude and frequency of the microcantilever motion. For that reason, the micro-cantilever supposedly oscillates according to:

$$z(t) = A(t) \sin(\omega_c t + \varphi_c(t)),$$

Equation 3 is also the input signal to the PLL, as it can be seen in Fig. 2.

### 2.2 The Amplitude Detector

The amplitude $A(t)$ of the micro-cantilever and tip oscillation is obtained by a circuit composed of a diode followed by a first-order low pass filter as shown in Fig. 4.

![Fig. 4. The amplitude detector.](image)

and the mathematical model of the amplitude detector is given by:

$$\dot{A}(t) + \tau_d A(t) = \tau_d z_d(t),$$

where $\tau_d = \frac{1}{RC}$, and

$$z_d(t) = \begin{cases} z(t), & z(t) > 0 \\ 0, & z(t) \leq 0. \end{cases}$$

### 2.3 The PLL mathematical model

The PLL is a closed loop control system composed of a phase detector (PD), a low-pass filter $f(t)$ and a voltage controlled oscillator (VCO), that synchronizes the local VCO output to the input signal $z(t)$ (Fig. 3). This is performed by

In the FM-AFM the tip and sample interactions generate frequency shifts [2].
adjusting the VCO frequency according to \( v_c(t) \), which in turn is the filter response to the PD output \( v_d(s) \). The output signal is given by:

\[
v_o(t) = v_o \cos(\omega_c t + \varphi_o(t)),
\]

where \( \varphi_o \) is the estimative of the loop to the input phase \( \varphi_c \) (see eq. 3), \( v_o \) is the amplitude of the output signal. Since both input and output signals are supposed to have the same central frequency \( \omega_c (\text{rad/s}) \), the phase error is defined as follows:

\[
\vartheta(t) = \varphi_c(t) - \varphi_o(t).
\]

Since the AGC keeps the microcantiler amplitude constant, the only parameter that can react to tip and sample forces is the change of the resonant frequency. This shift of frequency is detected and used to change the distance \( d \) (Fig. 1), in order to generate topographic images [3]. Consequently, for design and analysis purposes, the input \( \varphi_c \) to the PLL can be written as:

\[
\varphi_c(t) = \Omega t.
\]

The PLL is described by a differential equation of order \( P+1 \) [9], considering that the order the filter \( f(t) \) is \( P \). The filter transfer function is given by:

\[
F(s) = \sum_{m=0}^{M} \frac{\alpha_m s^m}{\sum_{p=0}^{P} \beta_p s^p}.
\]

The PD output is given by:

\[
v_d(t) = k_m v_i(t) v_o(t),
\]

where \( k_m \) is the PD gain.

The VCO frequency is controlled according to:

\[
\dot{\varphi}_o(t) = k_o v_c(t),
\]

where \( k_o \) is the VCO gain, and \( v_c \) is the filter output given by the convolution:

\[
v_c(t) = f(t) * v_d(t).
\]

The loop gain \( G \) is defined as follows:

\[
G = \frac{1}{2} k_m k_o v_o A_c.
\]

Considering the foregoing relations, the convolution theorem [13] and the trigonometric identity \( \sin(A) \cos(B) = \frac{1}{2} [\sin(A-B) + \sin(A+B)] \), the dynamics of the phase error is given by:

\[
L[\dot{\vartheta}] + GQ \left[ A(t) (\sin(\dot{\vartheta}(t)) + \sin(2(\omega_c t + \varphi_c(t)) - \vartheta(t))) \right] = L[\varphi_o(t)]
\]

The trigonometric identity is applied into equation 10 in order to transform the product of trigonometric functions into a sum. The term with \( \sin(A-B) \) yields the phase difference term, and the term with \( \sin(A+B) \) yields the double frequency term.
where \( A(t) = \frac{A(t)}{A} \). The operators \( Q \) and \( L \) depend on the filter transfer function (Eq. 9), and are given by:

\[
Q[\cdot] = \sum_{m=0}^{M} \alpha_m \frac{d^m \cdot}{dt^m}, \quad (15)
\]

\[
L[\cdot] = \sum_{p=0}^{P} \beta_p \frac{d^{p+1} \cdot}{dt^{p+1}}, \quad (16)
\]

**Second-order Sallen-Key filter**

The filter considered is a second-order Sallen-Key filter shown in Fig. 5, with transfer function given by:

\[
F(s) = \frac{\mu\omega_n^2}{s^2 + \frac{\omega_n^2}{Q}s + \omega_n^2} \quad (17)
\]

with

\[
\omega_n^2 = \frac{1}{R_1R_2C_1C_2}, \quad (18)
\]

\[
Q = \frac{1}{\omega_n [C_2(R_1 + R_2) + R_1C_1(1-\mu)]}, \quad (19)
\]

and

\[
\mu = 1 + \frac{R_A}{R_B}. \quad (20)
\]

For \( R_1 = R_2 = R \) and \( C_1 = C_2 = C \) in equations 17 to 20, the transfer function of the "equal component" Sallen-Key filter [14] becomes:
\[ F(s) = \frac{\mu \omega_n^2}{s^2 + (3 - \mu) \omega_n s + \omega_n^2}. \]  

(21)

### 2.4 The complete FM-AFM control system model

Considering what was shown above the complete model of the FM-AFM is given by the following set of equations:

\[ \ddot{z}(t) + \gamma \dot{z}(t) + \omega_n^2 z(t) = r(t)v_o \sin{(\omega_c t + \varphi_o(t))} + \frac{A_H}{6(d(t) + z(t))^2}, \]  

(22)

\[ \dot{A}(t) + \tau_d A(t) = \tau_d z_d(t), \]  

(23)

\[ \ddot{\vartheta} + (3 - \mu) \omega_n \dot{\vartheta} + \omega_n^2 \dot{\vartheta} + \mu \omega_n^2 G(\Lambda(t)) \sin{\vartheta} = \omega_n^2 \Omega, \]  

(24)

\[ r(t) = \Phi_{AGC} (A_c - A(t)), \]  

(25)

\[ d(t) = \Phi_{ADC} (\Delta \omega_c - \dot{\varphi}_0(t)). \]  

(26)

where Eqs 22, 23 and 24 are the micro-cantilever, amplitude detector and PLL mathematical models, respectively. Additionally, equations 25 and 26 are the control law for the AGC and ADC systems, respectively.

In Equation 24, the double frequency term was dropped since it is supposed to be cut by the low pass filter, however, the double frequency jitter is always present, and depending on the system requirements it must be considered [9,10,12].

### 3 PLL lock-in range

Equation 24 represents the dynamics of a third-order PLL on a cylindrical phase surface, i.e., a complete analysis of the PLL behavior can be performed considering \( \vartheta \in (-\pi, \pi] \). In this case the synchronous state corresponds to a constant phase error \( \vartheta \) and null frequency and acceleration errors \( \dot{\vartheta} = \ddot{\vartheta} = 0 \) for \( t > t_s \) [7,12,15].

The lock-in range for the Sallen-Key third-order PLL is composed of the set of the values of the loop gain \( G \), of the filter gain \( \mu \), of the filter cutoff frequency \( \omega_n \) and of the microcantilever resonant frequency shift \( \Omega \) for which equation 24 presents an asymptotically stable synchronous state \( (\vartheta, \dot{\vartheta}, \ddot{\vartheta}) = (\vartheta^*, 0, 0) \) with \( \vartheta \in (-\pi, \pi] \). In this case it is considered that \( \Lambda(t) = 1 \) for all \( t \). The lock-in range can be determined with the bifurcation analysis of equation 24, which can be transformed into state space equations by defining:
\[ \begin{align*}
x_1 &= \vartheta(t) \\
x_2 &= \dot{\vartheta}(t) \\
x_3 &= \ddot{\vartheta}(t)
\end{align*} \]

resulting in

\[ \begin{align*}
\dot{x}_1 &= x_2 \\
\dot{x}_2 &= x_3 \\
\dot{x}_3 &= \omega_n^2 \Omega - (3 - \mu)\omega_n x_3 - \omega_n^2 x_2 - \mu \omega_n^2 G \sin(x_1).
\end{align*} \]

The Jacobian matrix is given by:

\[
J \bigg|_{x_1 = x_1^*} = \begin{bmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
-\mu \omega_n^2 G \cos(x_1^*) & -\omega_n^2 & -(3 - \mu)\omega_n
\end{bmatrix},
\]

and consequently, the characteristic polynomial by:

\[
P(\lambda) = \lambda^3 + (3 - \mu)\omega_n \lambda^2 + \omega_n^2 \lambda + \mu \omega_n^2 G \cos(x_1^*). \tag{30}
\]

For \( x_1 \in (-\pi, \pi], x_2 = x_3 = 0 \) and from equation 28 the equilibrium points can be determined by:

\[
x_1^* = \sin^{-1} \left( \frac{\Omega}{\mu G} \right). \tag{31}
\]

It can be seen from equation 31 that for

\[
|\Omega| > \mu G \tag{32}
\]

there is no synchronous state. Additionally, for \( |\Omega| = \mu G \), and from equation 30, there are two non-hyperbolic synchronous states, namely, \( \left( \frac{\pi}{2}, 0, 0 \right) \) and \( \left( -\frac{\pi}{2}, 0, 0 \right) \), for \( \Omega > 0 \) and \( \Omega < 0 \), respectively.

For \( |\Omega| < \mu G \) there are four synchronous states. Two for \( \Omega > 0 \), given by: \( x^{*1} = (x_1^{*1}, 0, 0) \) and \( x^{*2} = (\pi - x_1^{*1}, 0, 0) \); and another two for \( \Omega < 0 \), given by: \( x^{*3} = (-x_1^{*1}, 0, 0) \) and \( x^{*4} = (- (\pi - x_1^{*1}), 0, 0) \).

Since \( x^{*2} \) and \( x^{*4} \) are respectively located on the third and fourth quadrants, it follows from the Routh-Hurwitz criterion [16] and the characteristic polynomial (equation 30) that both are unstable for any parameters combination.

On the other hand, \( x^{*1} \) and \( x^{*3} \) can be stable or not, depending on the parameters combination. In addition, since \( \cos (x_1^{*1}) = \sqrt{1 - \left( \frac{\Omega}{\mu G} \right)^2} = \sqrt{1 - \left( \frac{x_1^{*3}}{\mu G} \right)^2} = \cos(-x_1^{*1}) = \cos (x_1^{*3}) \) the characteristic polynomial can be rewritten as:
\[ P(\lambda) = \lambda^3 + (3 - \mu)\omega_n\lambda^2 + \omega_n^2\lambda + \mu\omega_n^2 G\sqrt{1 - \left(\frac{\Omega}{\mu G}\right)^2}, \]  
(33)

and, consequently, the stability analysis performed on the characteristic polynomial of equation 33 is valid for both \[ x^{*,1} \] and \[ x^{*,3} \], i.e., for \( \Omega > 0 \) and \( \Omega < 0 \), respectively.

The stability of \( x^{*,1} \) and \( x^{*,3} \) can be determined by the Routh-Hurwitz criterion. Therefore, the Routh-Hurwitz matrix is written as follows:

\[
R = \begin{bmatrix}
1 & \omega_n^2 G\sqrt{1 - \left(\frac{\Omega}{\mu G}\right)^2} \\
(3 - \mu)\omega_n & \mu\omega_n^2 G\sqrt{1 - \left(\frac{\Omega}{\mu G}\right)^2} \\
\frac{(3 - \mu)\omega_n^2 - \mu\omega_n G\sqrt{1 - \left(\frac{\Omega}{\mu G}\right)^2}}{3 - \mu} & 0 \\
\mu\omega_n^2 G\sqrt{1 - \left(\frac{\Omega}{\mu G}\right)^2} & 0
\end{bmatrix}.
\]

The synchronous states \( x^{*,1} \) and \( x^{*,3} \) are asymptotically stable if all elements in the first column of \( R \) are positive. Consequently, \( \mu \) that is greater than 1, due to the construction of the filter, must be lower than 3, or concisely:

\[ 1 < \mu < 3. \]  
(34)

In addition, \( (3 - \mu)\omega_n^2 - \mu\omega_n G\sqrt{1 - \left(\frac{\Omega}{\mu G}\right)^2} \) must be positive, and for physical meaningful parameters, it results that:

\[ G < \frac{1}{\mu} \sqrt{(3 - \mu)^2\omega_n^2 + \Omega^2}. \]  
(35)

Inequality 34 defines the lower and upper bounds for the lock-in range of the filter gain \( \mu \), and inequality 35 defines the upper bound of the loop-gain \( G \). The Lower bound of \( G \) is defined by the synchronous states existence condition (equation 32), resulting that:

\[ G \geq \frac{|\Omega|}{\mu}. \]  
(36)

The inequalities 34, 35 and 36 define the lock-in range for the Sallen-Key third-order PLL. For design purposes the lock-in range must be defined for \( \Omega = \Omega_{\text{max}} \), i.e., the maximum microcantilever resonant frequency shift possible for a given scanning of a sample. As an example, Figs. 6 and 7 show the lower bound of the lock-in range and the lock-in range for \( \Omega = \Omega_{\text{max}} = 200\pi\text{rad/s} \) (100Hz).

The existence of the synchronous states is determined by a saddle-node bifurcation, represented by the lower bound of the lock-in range. For parameter values lower than the critical value, there are no equilibrium solutions, i.e., a constant phase error \( \vartheta \) and null frequency and acceleration errors \( \dot{\vartheta} = \ddot{\vartheta} = 0 \) for \( t > t_s \) [7,12,15]. On the other hand, for parameter values higher than the
critical values, there are four hyperbolic equilibrium solutions, two stable, and two unstable.

The upper bound of the lock-in range is given by a Hopf bifurcation, generating a family of periodic solutions (limit-cycles) for loop gains above the upper

Fig. 6. Lower bound of the lock-in range for the third order Sallen-Key PLL

Fig. 7. Lock-in range for the third order Sallen-Key PLL
bound [7,17]. Therefore, combining the lower bound, given by the saddle-node bifurcation, with the upper bound, given by the Hopf bifurcation, it can be concluded that the lock-in range for the third order PLL with second-order Sallen-Key filter is represented by the region between the two surfaces as shown in Fig. 7.

4 Simulations results

In this section some simulation results are presented in order to illustrate the PLL behavior concerning the lock-in range and the frequency demodulation process. The simulations are performed built-in Simulink blocks, using the 4th order Runge-Kutta integration algorithm. The central frequency $\omega_c$ is $200\pi \times 10^3 \text{rad/s}$ (100kHz).

The loop filter used in the simulation is a Butterworth Sallen-Key filter [14] with parameters set to $\omega_n = \frac{\omega_c}{100}$ and $\mu = 1.5858$. In accordance with inequality 35 and for $\Omega = \Omega_{\text{max}} = 200\pi\text{rad/s}$ it results that $G_{\text{max}} < 5.6174 \times 10^3$, and from inequality 36 $G_{\text{min}} > 396.2189$. The simulations results are shown in Figs. 8, 9 and 10.

The simulations results in Fig. 8 show the response of the PLL operating inside the lock-in range. Figs. 8(a), 8(c) and 8(e) show the phase error response for $G = G_{\text{min}}$, $G = 0.4G_{\text{max}}$ and $G = 0.8G_{\text{max}}$, respectively. Since the PLL designed is a type 1 system it presents steady state phase error and, as expected, the bigger the loop gain $G$ the lower the steady state error.

Likewise, Figs. 8(b), 8(d) and 8(f) show the frequency demodulation response of the PLL to the FSK signal with amplitude $\Omega_{\text{max}}$, for $G = G_{\text{min}}$, $G = 0.4G_{\text{max}}$ and $G = 0.8G_{\text{max}}$, respectively. It can be noticed that the bigger the loop gain $G$ the more oscillatory the frequency demodulation response. On the other hand, the settling time is bigger for loop gains set near the boundaries of the lock-in range.

Fig. 9 show simulations responses to loop gains above the upper bound of the lock-in range. Since the upper bound represents a Hopf bifurcation Figs. 9(a) and 9(b) show the onset of a limit-cycle [17]. Additionally, the limit-cycle amplitude increases over the loop gain $G$.

In addition, Fig. 10 show the simulations responses for loop gains $G$ set below the lower bound of the lock-in range. The lower bound represents the saddle-node bifurcation and, as mentioned earlier, it indicates that below this boundary there are no synchronous states. Accordingly, in Fig. 10(a) it can be seen that the phase error increases over time, also, in Fig. 10(b) it is clear that the FSK signal $\Omega_{\text{max}}$ is not properly demodulated.

5 Conclusion

The PLL performance is vital to the FM-AFM and, accordingly, it must be properly designed in order to assure the correct demodulation of the tip and...
sample interactions from the microcantilever motion. Here, the lock-in range for a third-order PLL with second-order Sallen-Key filter is determined, and simulations supporting the theoretical results are shown, giving hints on how to determine the PLL parameters in order to assure the existence of synchronous states, and how to improve the PLL performance.

Fig. 8. Simulations with \( G_{\text{min}} \leq G < G_{\text{max}} \).
Fig. 9. Simulations with $G \geq G_{\text{max}}$.

Fig. 10. Simulations with $G < G_{\text{min}}$.

References


Using Average Mutual Information to Preview the Power Spectrum and to Guide Nonlinear Noise Reduction

N. Jevtic\textsuperscript{a,b}, W. Nilsen\textsuperscript{a}, P. Stine\textsuperscript{a}, J. S. Schweitzer\textsuperscript{b}

\textsuperscript{a} Bloomsburg University, 400 Second St, Bloomsburg, PA 17815, USA
\textsuperscript{b} Physics Department, University of Connecticut, Storrs, CT 06269, USA

Abstract: Power spectra of nonlinear time series often contain relevant information across all frequencies. Traditional filtering results in loss of information at the high frequencies. Nonlinear local projective noise reduction is a method that allows us to reduce noise while retaining high-frequency information. Results for two quasi-periodic stars, a variable white dwarf and a period-doubling star, are discussed. For both, we show that average mutual information (AMI) allows us to preview the power spectrum including at higher frequencies in the white-noise tail. Once a power spectrum is obtained, AMI can also serve as an indicator of the limits to which nonlinear noise reduction can be taken.

Keywords: Nonlinear time series analysis, Power spectrum, Average mutual information, Nonlinear noise reduction, Variable stars

1 Introduction: Phase-space Portrait and the Parameters of the Time-Delay Reconstruction

One of the tools to explore nonlinear systems is a time-delay phase-space portrait. According to the embedding theorems \cite{10, 8, 9}, the geometry of this time-delay phase-space portrait is diffeomorphic to the geometry of the phase-space representation that would be obtained if the equations governing the system were known. Thus, this object is a surrogate and can be studied in lieu of the system.

To obtain a time-delay phase-space portrait of a uniformly-sampled time series, the parameters of the reconstruction have to be determined first. These are the phase-space dimension and the time delay, which are both obtained from the data.

1.1 Dimension of the Phase Space

The dimension of the reconstructed phase space is obtained using the False Nearest Neighbour (FNN) method \cite{7} on the time series itself. This dimension is important because it is related to the number of degrees of freedom needed to model the system.
1.2 Time Delay

Autocorrelation Function

Historically the choice of the time delay was initially made using the autocorrelation function. Given N observations \(s_1, s_2, s_3, s_4, \ldots\) at times \(t_1, t_2, t_3, t_4, \ldots\) the autocorrelation lag \(\tau\) is given by:

\[
C(\tau) = \frac{1}{N-\tau} \sum_{i=1}^{N-\tau} (s_i - \bar{y})(s_{i+\tau} - \bar{y})
\]

Here \(\bar{y}\) is the mean and \(\sigma\) is the standard deviation. The autocorrelation function quantifies the similarity between observations as a function of the time separation between them. The options for the time delay are the correlation time, the zero or the minimum of the autocorrelation function.

Average Mutual Information

Over time the trend has been to choose the optimal time delay at the minimum of average mutual information [3]. Average mutual information (AMI) is an information-theory analog to the autocorrelation function. AMI is defined in terms of probabilities as:

\[
AMI(\tau) = \sum_{i,j} p_{i,j} \log_2 \left( \frac{p_{i,j}}{p_i p_j} \right)
\]

AMI is the amount of information (in bits) shared by the signal and its time shifted value averaged over the orbit. It is a measure of how much one learns from one signal about the other.

For a uniformly sampled time series such as a stellar light curve AMI is:

\[
AMI(\tau) = \sum_{s(t), s(t+\tau)} P(s(t), s(t+\tau)) \log_2 \left( \frac{P(s(t), s(t+\tau))}{P(s(t))P(s(t+\tau))} \right)
\]

Here \(s\) is the sampled scalar time series and \(\tau\) is the time delay. The range of the time series is divided into \(m\) sub-intervals and a histogram is obtained that yields the probability \(p_i\) for a point to be in the interval \(i\), the probability \(p_j\) for a point to be in the interval \(j\), and the joint probability \(p_{i,j}\) that if \(s_k\) is in interval \(i\) then \(s_{k+\tau}\) is in interval \(j\).

Whether the first, local minimum, or the global minimum best determine the optimal delay is still a point open to discussion.
Though AMI is analogous to the autocorrelation function of linear signal processing, it is more general in the statistical sense since the autocorrelation is the expectation of a quadratic polynomial statistic, while AMI represents the expectation of the average degree of independence incorporating all higher orders. Though AMI was initially used to obtain the optimal time delay for time-delay embeddings its probabilistic nature gives it wider applicability [2].

2 Locally-projective nonlinear noise reduction

The measured data are assumed to be the output of a low-dimensional dynamical system and random high-dimensional noise. This noise spreads the data off its manifold in phase space. For small amplitude noise, it is assumed the data are distributed closely around the manifold [4, 5].

In order to reduce noise it is therefore important to first identify this manifold and then to orthogonally project the data points onto it. For a trajectory whose delay vectors \( a_n \) lie inside a \( m \)-dimensional manifold, while the dynamical system with noise forms a \( q \)-dimensional manifold where \( q > m \). To reduce noise we over-embed and repeat the process until, due to iteration, the average correction ceases to decrease rapidly. An example of the application of the method is detailed in Jevtic et al. [6].

However, reducing noise in signals from nonlinear systems poses unique challenges. Most nonlinear systems have broadband power spectra. Differentiating noise from signal in such spectra is difficult if not impossible. It would be to great advantage if the shape of the spectrum buried by noise were known. Moreover, in such spectra, over-reduction can result in spurious results. An indication when to stop nonlinear noise reduction would greatly reduce the generation of spurious results. We will show that average mutual information can be used to advantage in both of these cases.

3 Requirements on the data

At this time, nonlinear phase-space reconstruction can only be used for uniformly-sampled continuous data sets.

4 Data Analysis

The light-curve data for two quasi-periodic stars are analysed. For a variable white dwarf and a period-doubling star we show that average mutual information (AMI) is a better predictor of the power spectrum since it can preview what is under the noise. It can also serve as a guide to when to stop nonlinear noise reduction to guard against spurious results. For the period-doubling star for which long continuous light curves are available, phase-space portraits and power spectra are investigated for sub-intervals over time.
DB White Dwarf PG1351+489

Eleven hours of continuous DB white dwarf PG1351+489 data were analysed [6], Fig. 1. This section of the light curve was obtained by the ground-based Whole Earth Telescope international collaboration during its xCov12 campaign.

The autocorrelation function (black curve) and the Average Mutual Information (AMI) (red curve) for the above data are shown in Fig. 2. The two curves are scaled to the first maximum. The correlation function (red curve) indicates the presence of only a single periodicity. The AMI (black curve) indicates a “primary” comb of a fundamental and harmonics whose magnitude diminishes
with delay. A “secondary” comb of sub-harmonics is also present between the “primary” ones which has constant magnitude.

Fig. 3 PG 1351+489 power spectra before (gray) and after noise reduction (black)

Power spectra for white dwarf PG 1351+489 before (gray) and after noise reduction (black) are shown in Fig. 3 for ~11h of data. The black power spectrum is after noise reduction from 7 dimensions with 6 iterations. The white-noise tail is lowered by a factor of ~50. More lines were identified than from the whole xCov12 run of 84 h [1]. Thus noise reduction allows us to shorten the data-collection time by a factor of 7.

In both power spectra, as predicted by AMI, a fundamental and its harmonics are present. Also, there is a comb of sub-harmonics. Moreover, the line amplitude diminishes with frequency.

**TYC 3544-1245-1**

The second star analysed is listed in the Tycho2 catalogue as TYC 3544-1245-1. Its light curve is shown in Fig. 4.
Fig 4. TYC 3544-1245-1 Light Curve

Though there is period doubling, the classification of this star is still being debated. At times it has been classified as a solar-like star, an RR Lyrae star, a delta Scuti star and a W UMa contact binary. However, for the purposes of this paper, behaviour not classification is important.

Fig. 5 Autocorrelation function (red) and Average Mutual Information (AMI) (black) for TYC 3544-1245-1
In Fig. 5 the correlation function (red curve) indicates the presence of a periodicity and its harmonics and a single sub-harmonic all of constant amplitude. The AMI (black) curve also indicates that the periodicities present consist of a “primary” comb consisting of a fundamental frequency and its harmonics but the single sub-harmonic has become a “secondary” comb of three smaller sub-harmonics between subsequent “primary” peaks. The amplitudes of the “primary” comb diminish with delay while the amplitudes of the “secondary” comb remain constant.

Fig. 6 The power spectrum of three months of data for TYC 3544-1245-1

The power spectrum of three months of TYC 3544-1245-1 data is shown in Fig. 6. This spectrum has a significant noise contribution and widened line bases. It does not agree with the “prediction” of the AMI.

Fig. 7. TYC 3544-1245-1 phase-space portrait with evident changes in the dynamics
However, the phase-space portrait for the same period (Fig. 7) indicates that behaviour changed over time. As a result the data were divided into one month intervals and the last month was further subdivided into two fifteen-day segments. The results of nonlinear projective local noise reduction for the two last month two fifteen-day segments are shown in Fig. 8.

![Power Spectra Comparison](image)

**Fig. 8** Comparison of the power spectra for the two consecutive 15-day intervals after noise reduction: blue - 1st interval (top); red - 2nd interval (bottom).

The power spectra after nonlinear noise reduction for the two fifteen-day intervals are compared in Fig. 8. Noise reduction was considerably more efficient for the second. For the 2nd fifteen-day interval the AMI prediction of a comb of primary frequencies of diminishing amplitude with delay, and a triplet of smaller sub-harmonics between primary peaks can be seen to be correct. However, the number of “primary” harmonics that can be identified has not increased.

Since the red power spectrum for the second 15 days can be interpreted as a change in the dynamics, the search for an explanation led to a second inspection of the phase-space portraits of the two 15-day intervals separately.
Noise reduction was much more efficient for the second (red) segment that has a more developed surface in phase space due to de-threading. Thus we observe all the frequencies predicted by AMI due to an interplay of a moderate parameter change and the nature of that change that allows for efficient noise reduction. A second noise reduction resulted in the power spectra shown in Fig. 10.

The power spectra of the two 15-day data sets after a second round of nonlinear noise reduction in Fig. 10 are an illustration of another aspect of the utility of AMI.
For the second interval power spectrum (rendered in green), the number of accessible “primary” harmonics has increased dramatically. However, the “triplet sub-comb” predicted by AMI has been considerably suppressed at the higher frequencies. If the bottom (2nd interval-green) spectrum is compared with the top (1st interval-violet) 15-day power spectrum in Fig. 10, at the higher frequencies the onset of the region in which the triplets are over-suppressed in the bottom (green) spectrum corresponds to the onset of spurious structures in the top (violet) spectrum. Thus, AMI can also be used to estimate when noise reduction should be stopped to avoid the introduction of artefacts. In practice, fewer iterations will protect against this.

5 Conclusions

Average Mutual Information (AMI) remains the most effective tool to select the optimal delay for time-delay phase space reconstruction. Earlier work [2] demonstrated the predictive value of a variant of average mutual information in the time domain. In the frequency domain, for quasi-periodic light curves, we show that AMI is a much more powerful tool than generally appreciated. For the light curves considered, AMI over a range of delays previews the shape of the Fourier power spectrum with fidelity even when there is considerable white noise present.

Moreover, as complexity grows with the increase of the number of sub-harmonics present the autocorrelation function, the AMI linear analog, continually underestimates the multiplicity of sub-harmonics. Even without a definitive, more extensive study of a variety of light-curve shapes, it is safe to say, by analogy, that AMI yields a reliable estimate for the lower bound on the multiplicity of sub-harmonics.

A preview of the power spectrum is a major advantage when reducing noise in signals from nonlinear systems which have broadband power spectra. Differentiating noise from signal in such spectra is difficult if not impossible. However, there is an additional benefit in that AMI also allows us to set limits on when noise reduction should be stopped since over-reduction may lead to spurious results. Knowing when noise reduction starts suppressing parts of the power spectrum that are actually integral to it and needed to model the dynamics is also extremely valuable.

Of the two light curves used to illustrate this new approach to AMI, the TYC 3544-1245-1 data proved to be the more interesting. Period doubling was detected for TYC 3544-1245-1. In addition, the phase-space portrait for two successive intervals indicated a moderate change in dynamics that resulted in de-threading [6] leading to a surface that allows for more efficient noise reduction. Nonlinear noise reduction for that part of the light curve resulted in a power spectrum predicted by the AMI consisting of a “primary” fundamental, its harmonics and a “secondary” sub-harmonic triplet structure between them. Moreover, even though repeated noise reduction resulted in better access to the “primary” harmonics, it proved excessive at higher frequencies suppressing the
“secondary” triplet structure. This can practically be easily remedied by using a smaller number of iterations.

To our knowledge, no other method gives as good a preview of the power spectrum in the presence of considerable noise. Also, though not quantitative as yet, AMI promises to develop into a useful tool to delineate useful from artefact-generating noise reduction.

References

1. V.M. Alves et al., The Pulsating DB White Dwarf PG 1351+489, 2003, Baltic Astron., 12, 33

Acknowledgements

The WET for the PG1351+489 data: the xCov12 campaign team, particularly Antonio Kanaan and Steve Kawaler.

For the publically available data, we thank the entire Kepler team for the development and operations of this outstanding mission and all involved in KASC for the handling of the data. Their efforts have allowed us to conduct the theoretical work on nonlinear time series methodology presented herein. Funding for the Kepler Mission is provided by NASA’s Science Mission Directorate.

The Bloomsburg University Faculty Travel Fund and the Bloomsburg University Foundation.

Electron-electron Collisions and Drift Velocity
Fluctuations in n-GaAs at T=80 K

Romas Raguotis
Centre of Physical Sciences and Technology Semiconductor Physics Institute,
Vilnius, Lithuania
E-mail: romasr@pfi.lt

Abstract: Modified combined scattering rate Monte Carlo technique is proposed. Electron collisions with phonons, impurities and among themselves are taken into account. The proposed technique avoids the short-time-step procedure inherent to conventional ensemble Monte Carlo method. All \(N\) modelled electrons move using the total probability for the scattering of each electron by the thermal bath and mutual scattering between electrons pairs (“events in the electron system”). The quantitative fitting to the available experimental data on the spectral density is achieved and the range of moderate fields is defined for interparticle collisions to manifest themselves in the noise. In the second part of the presented report a drift velocity correlator is investigated numerically by Monte Carlo simulation and for the first time analytically by a phenomenological approach taking into account electron-phonon and electron-electron scattering between free carriers. The thermodynamic approach is investigated. The results of the velocity-to-velocity correlation functions and electron noise spectrum obtained analytically are in quite good agreement with those given by the Monte Carlo method.

Keywords: Monte Carlo, Electron-electron collisions, Drift velocity fluctuations, Spectral density.

1. Introduction
Fluctuations phenomena in semiconductors have been intensively investigated during the last three decades [1-3]. Fluctuation effects have been conventionally investigated without an account on the Coulomb electron-electron (e-e) scattering. However at sufficiently high electron densities, it is necessary to take into account e-e scattering to the total distribution function and related correlators.

Interparticle collisions though conserving energy and momentum of the electron system have an indirect effect on transport and – even more direct – on velocity correlations. In the presented report the ‘combined scattering method’ (CSR) Monte Carlo method [4] is used to interpret the results of microwave noise.

The important role of e-e collisions is demonstrated, and drift-velocity to drift-velocity cross-correlation under non-equilibrium conditions is calculated. In the second part drift velocity correlation functions are investigated analytically in a...
phenomenological approach and numerically through Monte Carlo simulation. Thermodynamic equilibrium state is investigated. Analytical results are in good agreement with those obtained by Monte Carlo method in the GaAs crystal.

2. Electron-electron collisions. Drift velocity fluctuations

It can be shown [4] that the “time of free flight” for independent scattering events of the \( N \) electron system with \( k \) wave-vectors is defined by the combined scattering rate:

\[
\lambda_{\text{comb}}(k_1, k_2, ..., k_N) = \sum_{i=1}^{N} \lambda_i(k_i) + \frac{1}{N-1} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \lambda_{ij}^{ee}(k_i, k_j),
\]

where \( \lambda_i(k_i) \) and \( \lambda_{ij}^{ee}(k_i, k_j) \) are conventional integral rates of scattering of the \( i \)th electron by the thermal bath and by the \( j \)th electron respectively [5]. Equation (1) reduces to that written down in [6] for \( N=2 \). All \( N \) electrons move without scattering for the “time of free flight of the system” between two successive events of an electron scattering by the thermal bath or mutual collision between two electrons occurs. The “time of free flight” is defined from the sum of the each electron scattering rate on the thermal bath and on the all remaining electrons. CSR technique avoids the short-time step procedure and a large electron number inherent to conventional ensemble MC simulation.

The time-displaced drift-velocity correlation function is

\[
\Phi_{\text{total}}(t) = N \Phi_{\text{total}}(t+t) = \Phi_{\text{auto}} + \Phi_{\text{cross}},
\]

where the auto- and cross-correlation functions are defined as:

\[
\Phi_{\text{auto}} = \frac{1}{N} \sum_{i} \delta v_i(t_1 + t) \delta v_i(t_1), \quad \Phi_{\text{cross}} = \frac{1}{N} \sum_{i \neq j} \delta v_i(t_1 + t) \delta v_j(t_1),
\]

In order to demonstrate the effect of e-e collisions on fluctuations, the calculated velocity correlation functions in a heating electric field are shown in Figure 1 for the model corresponding to n-type GaAs with the impurity scattering neglected. In our case \( \tau_{ee} \leq \tau_p \), strong cross-correlation appears. The equal-time cross-correlation also appears in non-equilibrium system as it was predicted in [1]. The auto-correlation decreases mainly in time \( \tau_{ee} \). The decay of \( \Phi_{\text{total}} \) is caused by the electron interaction with thermostat. In thermodynamic equilibrium, when \( \Phi_{\text{cross}}(0) = 0 \), the latter is equal to \( \Phi_{\text{total}}(0) = \Phi_{\text{auto}}(0) = V^2 = kT / m \).
The results of the spectral density of drift velocity fluctuations are presented in Figure 2. The experimental data are obtained from the current fluctuations data through normalization at zero field by using mobility data and Nyquist formula [7]. One can see that the most pronounced effect is obtained at intermediate fields ranging from 5 V/cm to 500 V/cm.

The nearly constant behavior at fields up to 100 V/cm can be explained by enhanced energy loss by electrons on optical phonons in the presence of e-e collisions. The role of e-e collisions diminishes at higher field.
3. Drift velocity correlations in semiconductors in the thermodynamic equilibrium state.

The values of correlators at the thermodynamic equilibrium have been calculated for the parabolic model of Γ valley in GaAs. The material parameters correspond to those listed in [8]. Electron scattering on non-elastic acoustic and optical modes of lattice vibrations, as well as e-e scattering \( n_e = 10^{15}\) cm\(^{-3}\) is taken into account. Inter-electron collisions are treated in the Brooks-Herring approximation. Standard expressions for electron scattering rates are used [5]. The calculations are performed by the CSR MC method.

Let us start with the simplified Boltzmann-Langevin equation for the fluctuation distribution function. In the state of thermodynamic equilibrium it can be written as

\[
\frac{d\delta F_p(t)}{dt} = -\frac{\delta F_p(t)}{\tau_p} - \frac{\delta F_p(t) - \delta F_p^M(t)}{\tau_{ee}} + y_p(t) \tag{4}
\]

Here \( F_p(t) \) is the instantaneous electron momentum distribution function, \( F_p^M(t) \) is the drifted Maxwellian distribution corresponding to the \( F_p(t) \) at time \( t \), \( y_p(t) \) describes the Langevin random force. In our case the rate of fluctuation relaxation is governed by the lattice and e-e scattering mechanisms.

The first term on the right-hand side of equation (4) ensures the relaxation of instantaneous distribution \( F_p(t) \) to the equilibrium distribution during lattice relaxation time \( \tau_p \). The second term is written in accordance with the Gross-Bhatnager-Krook approach [9]. Its form is based on the property of the instantaneous electron distribution function to acquire symmetric form (the drifted Maxwellian distribution) in the e-e scattering time \( \tau_{ee} \) under the influence of e-e scattering. R. Liboff in his textbook [10] gives considerable attention to this approach (see also [11]). Electron momentum can be intensively scattered by impurity centres too, but the energy of electrons is conserved in this scattering process. Even in this simple approach we cannot predict the final distribution that will result under the influence of impurity scattering. Therefore, we will omit further the impurity scattering.

The term \( \delta F_p^M(t) \) describes the deviation of a drifted Maxwellian distribution.

E-e scattering does not tend to bring either \( F_p^M(t) \) or \( F_p(t) \) to the thermodynamic equilibrium, because the average energy and momentum do not change during e-e collisions. So, the drifted Maxwellian distribution is supposed to relax only under the influence of lattice scattering during the corresponding scattering time \( \tau_p \). Therefore, we have used \( \delta F_p^M(t) = \delta F_p^M(0) \exp(-t/\tau_p) \).
Then, we multiply the equation (4) by the initial distribution function fluctuation \( \delta F_p(t_1) \), and average the product. Let us denote the correlator \( \delta F_p(t_1) \delta F_p(t_1 + t) \) as \( \delta F_p(0) \delta F_p(t) \). Now we write the dynamic equation:

\[
\frac{d\delta F_p(0) \delta F_p(t)}{dt} = -\frac{\delta F_p(0) \delta F_p(t)}{\tau_p} - \frac{\delta F_p(0) \delta F_p(t) - \delta F_p(0) \delta F_p(0) \exp(-t/\tau_p)}{\tau_{ee}}
\]

The last term in Eq. (4) representing a random force, vanishes because this force is \( \delta \)--correlated in time. Initial fluctuations of an actual distribution and the drifted Maxwellian distribution are related in the following way:

\[
\delta F_p(0) = \delta F_p(0) + \Delta F_p(0)
\]

where \( \Delta F_p(0) \) is deviation between them. Because of the chaotic behaviour of \( \Delta F_p(0) \) we assume that

\[
\delta F_p(0) \delta F_p(0) = \delta F_p(0) \delta F_p(0)
\]

We are interested in the velocity-to-velocity correlators; therefore we multiply the equation (5) by \( V_i(0)V_j(t) \) and sum it up by \( p \) and \( p \). Finally, we obtain the phenomenological equation describing the relaxation of the total velocity-to-velocity correlator coefficient \( c_{total}(t) = c_{auto}(t) + c_{cross}(t) \) in the thermodynamic equilibrium:

\[
\frac{dc_{total}(t)}{dt} = -\frac{c_{total}(t)}{\tau_p} - \frac{c_{total}(t) - c_{total}(0) \exp(-t/\tau_p)}{\tau_{ee}}
\]

The first-order linear differential equations for the velocity-to-velocity correlator coefficients can be then written as

\[
\frac{dc_{auto}(t)}{dt} = -\frac{c_{auto}(t)}{\tau_p} - \frac{c_{auto}(t)}{\tau_{ee}}
\]

\[
\frac{dc_{cross}(t)}{dt} = -\frac{c_{cross}(t)}{\tau_p} - \frac{c_{cross}(t)}{\tau_{ee}} + \frac{\exp(-t/\tau_p)}{\tau_{ee}}
\]

Taking into account the known initial conditions [1] under equilibrium: \( c_{auto}(0) = 1 \), and \( c_{cross}(0) = 0 \), the correlation coefficients are given as
As it is seen the auto-correlation coefficient in equilibrium decreases exponentially with a combined relaxation time \( \tau_c = \tau_p \tau_{\text{el}} / (\tau_p + \tau_{\text{el}}) \). This result describes conventionally the relaxation of the probe particle velocity correlator. We obtain from the second equation that the cross-correlation coefficient tends to increase during the time \( \tau_{\text{el}} \), but then decreases to zero per lattice scattering time.

One can see an important result of the total correlation coefficient:

\[
c_{\text{total}}(t) = c_{\text{auto}}(t) + c_{\text{cross}}(t) = \exp\left(-t / \tau_p\right).
\]

This shows that it does not depend on e-e scattering.

The analytical dependencies calculated with equation (11) reasonably well coincide with those from the MC data (Fig. 3).

The characteristic time at which the cross-correlation function reached its maximum in the case of \( \tau_{\text{el}} \leq \tau_p \) is \( t_{\text{max}} \approx \tau_{\text{el}} \ln(1 + \tau_p / \tau_{\text{el}}) \). The more details of the correlation functions behavior (spectral density, etc.) can be found in [12].

4. Conclusions

The presented MC procedure was demonstrated to be an efficient tool for studying electron noise in the presence of e-e scattering. Taking them in accordance is crucial for explanation of experimental data on microwave noise in doped GaAs.

The results of analytical approach are in good agreement with the Monte Carlo simulation, what confirms the usefulness of our simple analytical model. Till
now only the single particle autocorrelation behaviour has been describe analytically in the textbooks of fluctuation phenomena (for example, see [13]).

References