Chaotic Pattern Recognition
Using the Adachi Neural Network Modified in a Small-World Way

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Abstract. The pioneering contribution of this paper is to design and implement a Neural Network (NN) that demonstrates chaotic Pattern Recognition (PR) properties, and where the network in and of itself is a “small-world” or “scale-free” network. The foundational NN that we employ for this is the Adachi Neural Network (AdNN). The latter is a fascinating NN which has been shown to possess chaotic properties, and to also demonstrate Associative Memory (AM) and PR, while variants of the AdNN have also been used to obtain other PR phenomena, and even blurring. The problem with the Adachi NN is that it is a fully-connected network requiring quadratic computations for the training. Our aim in this paper is to reduce the computations needed for the training significantly. The motivation for this is the fact that most “physical” networks including biological NNs and Internet networks have the properties of complex small-world or scale-free networks. To place the paper in the right perspective, we mention that in [1] we managed to reduce the AdNN’s computational cost significantly by merely using a linear number of computations by enforcing a Maximum Spanning Tree topology and a gradient search method. However, from the perspective of a network’s structure, very few real-life networks have a tree-shaped linearly-connected topology. The question we consider in this paper is whether we can reduce the degree of connections of each node to mimic the small-world or scale-free phenomena, more akin to “real” NNs. Simultaneously, we shall also attempt to ensure that the newly-obtained network still possesses strong PR characteristics. To achieve this, we first construct a small-world network by means of the so-called N-W model. We then address the problem of computing the weights for the new NN. This is done in such a manner that the modified small-world connection-based NN has approximately the same input-output characteristics, and thus the new weights are themselves calculated using a gradient-based algorithm. By a detailed experimental analysis, we show that the new small-world AdNN-like network possesses PR properties for appropriate settings. As far as we know, such a small-world AdNN has not been reported, and the results given here are novel.

Keywords: Chaotic Neural Networks, Chaotic Pattern Recognition, Adachi-like Neural Networks, Small-world Networks.

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1 Introduction

In this paper we shall attempt to design and implement a Neural Network (NN) that demonstrates chaotic Pattern Recognition (PR) properties. However, unlike the existing NNs that demonstrate chaotic PR phenomena, our newly-designed network, in and of itself, must be a “small-world” or “scale-free” network. To clarify the difference between chaotic PR systems and traditional PR systems, we mention the following: The goal of the field of Chaotic PR systems can be expressed as follows: We do not intend a chaotic PR system to report the identity of a testing pattern with a “proclamation” of the pattern’s class. Rather, what we want to achieve, on one hand, is to have the chaotic PR system give a strong periodic or more frequent signal when a pattern is to be recognized. Further, between two consecutive recognized patterns, none of the trained patterns must be recalled. Finally, and most importantly, if an untrained pattern is presented, the system must give a chaotic signal. This is analogous to how the brain works. Once a pattern is recalled from a memory location, the brain is not “stuck” to it, it is also capable of recalling other Associated Memory (AM) patterns. This ability to “jump” from one memory state to another in the absence of a stimulus is one of the hallmarks of the brain, and this is one phenomenon that a chaotic PR system has to emulate.

Adachi et al and Calitoiu et al have done a lot of ground-breaking work in this area [2–4], and we have built on these results in various avenues [3–6], including that of designing a NN that can yield ideal chaotic PR [7]. Generally speaking, the computational burden of the original AdNN and its variants [2–4] is quadratic, rendering them to be impractical machines. This is also true of most of the current NNs which possess a regular topology, e.g., a completely connected graph or a neighbor-coupled graph. In [1] we managed to reduce the AdNN’s computational cost significantly by merely using a linear number of computations by enforcing a Maximum Spanning Tree topology and a gradient search method. All of these must be contrasted with “real” NNs which usually have irregular topology, e.g., a small-world or a scale-free graph. In our previous paper [6], we succeeded in creating a Random-AdNN by using the E-R model. Then we computed the weights for the new network by means of gradient search. The newly obtained network was shown to still possess PR and AM properties. The contribution of this paper is to present a novel NN which is connected in a small-world way, which we shall refer to as “Smallworld-AdNN”. This is achieved by using the N-W model followed by an effective gradient search strategy, whence the computational burden can be significantly reduced. Further, as we shall show presently, the Smallworld-AdNN is almost as effective as the fully-connected AdNN with regard to its chaotic and PR characteristics.

2 Designing the Smallworld-AdNN

2.1 The Topology of the Smallworld-AdNN

As mentioned above, to design the Smallworld-AdNN, we shall first arrive at a topology with edges connected in a small-world manner, by using the W-S
model. The second step will involve the computation of the weights associated with this new structure, which is an issue addressed subsequently.

There are many ways to generate a small-world NN. In this paper, we only utilize the Watts-Strogts (W-S) [8] and the Newman-Watts (N-W) models [9].

The general steps of the obtaining a W-S model are as follows:
1. Arrange the neurons in a cycle, and index them from 1 to \( N \).
2. Create a neighbor-coupled network, where each neuron is connected with \( k/2 \) neurons on both its sides. Thus, the degree for each neuron is \( k \).
3. Re-connect each edge of the network with fixed probability \( pr \). That is, for each edge, delete it with a probability \( pr \) and connect it with another randomly chosen neuron.

The reader will observe two special situations that arise from this W-S model: The new network becomes a random network if \( pr = 1 \) while it remains the same if \( pr = 0 \).

Obviously, the W-S model has the potential of causing some neurons to become isolated. In [9], Watts and his coauthor improved the W-S model by edge addition instead of deletion. Thus the second step is modified as follows: Randomly connect two unconnected neurons with a fixed probability \( pr \). Again, one can then see that if \( pr = 1 \), the network becomes fully connected while it remains the same if \( pr = 0 \). It is worth pointing out that the W-S and N-W are essentially the same when \( pr \) is small and the number of neurons, \( N \), is large.

In this paper, we shall use the N-W model to create a small-world network. Consequently, we build the topology of the Smallworld-AdNN by invoking the following algorithm.

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**Algorithm 1 Topology Smallworld-AdNN**

**Input:** \( N \), the number of neurons in the network, and a set of \( p \) patterns which the network has to “memorize”.

**Output:** The topology and initial weights of the Smallworld-AdNN.

**Method:**
1. Create a neighbor-coupled graph, \( G \), with \( N \) vertexes which is to represent the AdNN.
2. Connect two randomly chosen unconnected neurons with a fixed probability \( pr \).
3. Compute the initial weights of the edges of \( G \), \( \{ w_{ij} \} \), by the following:
   \[
   w_{ij} = \frac{1}{p} \sum_{s=1}^{p} (2x_s^i - 1)(2x_s^j - 1),
   \]
   where \( x_s^i \) is the \( i^{th} \) component of the \( s^{th} \) stored pattern.
4. If there is no edge between vertex \( i \) and \( j \), then let \( w_{ij} = 0 \);

**End Algorithm Topology Smallworld-AdNN**

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2.2 The Weights of the Smallworld-AdNN: Gradient Search

Since we have successfully created the structure of the Smallworld-AdNN by using the N-W model, it is clear that the NN at hand will not adequately compare with the original AdNN. Thus, our next task is to determine a new set of weights so as to force the Smallworld-AdNN to retain some of its PR
properties, namely those corresponding to the trained patterns. We briefly explain below the process for achieving this.

The Smallworld-AdNN is defined by following equations:

\[ x^S_i(t+1) = f(\eta^S_i(t) + \xi^S_i(t)), \] (1)

\[ \eta^S_i(t+1) = k_f \eta^S_i(t) + \sum_{e_{ij} \in \mathcal{G}} w^S_{ij} x^S_j(t), \] (2)

\[ \xi^S_i(t+1) = k_r \xi^S_i(t) - \alpha x^S_i(t) + a_i, \] (3)

where \( \{w^S_{ij}\}, x^S_i, \xi^S_i \) and \( \eta^S_i \) are the weights, outputs, and state variables of the Smallworld-AdNN respectively, and have similar meanings to \( \{w_{ij}\}, x_i, \xi_i \) and \( \eta_i \) of the AdNN.

In order to find the optimal values of \( \{w^S_{ij}\} \), we define the square error between the original output of the AdNN and new output at the \( n \)th step:

\[ E_p = \frac{1}{2} \sum_{i=1}^{N} (x^{A,p}_i - x^{S,p}_i(n))^2, \] (4)

where \( x^{A,p}_i \) and \( x^{S,p}_i \) imply the outputs of the \( i \)th neuron when the \( p \)th pattern is presented to the AdNN network and the Smallworld-AdNN network respectively. The overall global error is defined by \( E = \sum_{p=1}^{P} E_p \) where \( P \) is the number of trained patterns.

In order to adjust \( w^S_{ij} \) to obtain the least global error \( E \), we consider the gradient, \( \Delta w^S_{ij} \), and move \( w^S_{ij} \) by an amount which equals \( \Delta w^S_{ij} \) in the direction where the error is minimized. This can be formalized as below:

\[ \Delta w^S_{ij} = -\beta \frac{\partial E}{\partial w^S_{ij}} = -\beta \frac{\partial \sum_{p=1}^{P} E_p}{\partial w^S_{ij}} = -\beta \sum_{p=1}^{P} \frac{\partial E_p}{\partial x^{S,p}_i(n)} \cdot \frac{\partial x^{S,p}_i(n)}{\partial w^S_{ij}} \]

\[ = \beta \sum_{p=1}^{P} (x^{A,p}_i - x^{S,p}_i(n)) \cdot \frac{1}{\varepsilon} \cdot x^{S,p}_i(n) \cdot (1 - x^{S,p}_i(n)) \cdot x^{S,p}_j(n), \] (5)

where \( \beta \) is the learning rate of the gradient search. The formal algorithm which achieves the update is given in Algorithm 2. The results of a typical numerical experiment which proceeds along the above gradient search are shown in Fig. 1 and 2. In these simulations, we have chosen the learning rate \( \beta \) to be 0.05 and \( pr = 0.5 \). Specifically, we catalogue our experiments for three cases, i.e., when \( k/2 = 4 \), \( k/2 = 6 \) and \( k/2 = 10 \) respectively.

The simulation results are shown in Fig. 1 and 2. If \( k/2 = 4 \), the average value of \( \Delta w^S_{ij} \) does not converge at 0, as shown in Fig. 1. However, as \( k/2 \) increases, e.g., \( k/2 = 6 \), \( \Delta w^S_{ij} \) converges to 0, as shown in Fig. 2 (a). If \( k/2 \) is even larger, \( \Delta w^S_{ij} \) also converges to 0 but at a faster rate, as shown in Fig. 2 (c). This phenomenon can be easily explained: The larger the value of \( k/2 \),

1 Please note that in all the three cases, the total error \( E \) does not converge to 0. This is because we have modified the structure of the AdNN. The new network cannot behave exactly the same as the original one, but can approximate it.
Algorithm 2 Weights Smallworld-AdNN

Input: The number of neurons, $N$, a set of $P$ patterns, and the initial weights $\{w_{ij}^S\}$ of the Smallworld-AdNN. These initial weights are $\{w_{ij}^A\}$ for the edges in the smallworld graph, and are set to zero otherwise. The parameters and the setting which we have used are the learning rate $\beta = 0.05$, $\varepsilon = 0.015$, $\alpha = 10$, $k_f = 0.2$ and $k_r = 1.02$.

Output: The weights $\{w_{ij}^S^*\}$ of the Smallworld-AdNN.

Method:

1: Compute the outputs of the Smallworld-AdNN corresponding to the $P$ trained inputs.
2: For all edges of the Smallworld-AdNN, compute $\Delta w_{ij}^S$ as per Equation (5). Otherwise, set $\Delta w_{ij}^S = 0$.
3: $w_{ij}^S \leftarrow w_{ij}^S + \Delta w_{ij}^S$.
4: Go to Step 1 until $E$ is less than a given value or $\Delta w_{ij}^S \approx 0$.

End Algorithm Weights Smallworld-AdNN

the more are the edges that the Smallworld-AdNN has, leading to a better-fitting effect. In practice, we have opted to choose $k_f/2 = 6$ to obtain a finer trade-off between the effect of the fit and the associated computational cost.

Fig. 1. The figure on the left shows the variation of the average of $\Delta w_{ij}^S$ (averaged over all values of $i$ and $j$) over the first 200 iterations of the gradient search scheme. The average converges to a value arbitrarily close to zero after 70 time steps. The figure on the right shows the variation of the global error over the same time frame. Observe that this quantity does not converge to zero.

The Lyapunov analysis of the Random-AdNN is also available, but omitted here in the interest of space. It can be found in [10].

3 Chaotic and PR Properties of the Smallworld-AdNN

We now briefly report the PR properties of the Smallworld-AdNN. These properties have been gleaned as a result of examining the Hamming distance between the input pattern and the patterns that appear in the output. In this regard, we mention that the experiments were conducted using the Adachi data set, as shown in Fig. 3.

In the ideal setting we would have preferred the Smallworld-AdNN to be chaotic when exposed to untrained patterns, and the output to appear period-
Fig. 2. The figures show the variation of the average of $\Delta w_{ij}^S$ and the global error over the same time frame. The degree of the connection is $k = 12$ (for (a) and (b)) and $k = 20$ (for (c) and (d)) respectively.

Fig. 3. The $10 \times 10$ patterns used by Adachi et al. The first four patterns are used to train the network. The fifth patterns are obtained from the corresponding fourth patterns by including 15% noise in (a) and (b) respectively. The sixth pattern is the untrained pattern.

ically or more frequently when exposed to trained patterns. Besides yielding this phenomenon, the Smallworld-AdNN also goes through a chaotic phase and a PR phase as some of its parameters change.

By studying Fig. 1 and 2 we see that if $k/2 = 6$, the Smallworld-AdNN can fit the original AdNN very well. Thus, we have set the parameters in Algorithm 1 to be $pr = 0.5$ and $K = 6$ so as to obtain a better trade-off effect. We summarize the results for the Smallworld-AdNN by using different settings of $pr$. The others parameters are: $k_f = 0.2$, $k_r = 1.02$, $\alpha = 10$, $\varepsilon = 0.015$, $\beta = 0.05$. The results are tabulated in Table 1.

From this table we clearly see that the Smallworld-AdNN is able to “resonate” the input patterns with corresponding output patterns. If P1 is the input, then the network outputs P1 accordingly, while at the same time, no other trained patterns appear in the output sequence. Even when a noisy pattern is presented to the system, e.g., P5, which is a noisy pattern of P4 with 15% noise, the network still “resonates” P4 instead of P5 in the output se-
Table 1. The frequency of the Hamming distance between the input and the output patterns for the Smallworld-AdNN. The probability \( p_r = 0.5 \) and \( k/2 = 6 \)

<table>
<thead>
<tr>
<th>( p_r = 0.5, k/2 = 6 )</th>
<th>Input Patterns</th>
<th>Retrieved Patterns</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P1</td>
<td>P2</td>
</tr>
<tr>
<td>P1</td>
<td>96</td>
<td>0</td>
</tr>
<tr>
<td>P2</td>
<td>0</td>
<td>376</td>
</tr>
<tr>
<td>P3</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>P4</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>P5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>P6</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Furthermore, if the input is an untrained pattern, e.g., P6, none of the trained patterns will be recalled. In this case, even the input pattern P6 itself, will be retrieved only a few times, as one can see is much less than the other diagonal numbers obtained when input is P1 – P4. In this regard, we comment that using the values of \( p_r = 0.5 \) and \( k/2 = 6 \) are good enough for PR, which also significantly minimizes the computational burden. Indeed, as one can see, the distribution for the degree of each vertex of the Smallworld-AdNN has the form:

\[
p(k) = \left( \frac{N}{k-6} \right) \left( \frac{3}{N} \right)^{k-6} \left( 1 - \frac{3}{N} \right)^{N-k+6}
\]

which is approximately a Poisson distribution, as shown in Fig. 4.

Fig. 4. The degree of each neuron obeys the Poisson distribution. From this figure we can see that most of the neurons have degree 8 or 9, which means that the computational load has been significantly reduced when compared to the original AdNN, which we know has a vertex degree of 99.

4 Conclusions

In this paper we have concentrated on the field of Chaotic Pattern Recognition (PR), which is a relatively new sub-field of PR. Such systems, which have only recently been investigated, demonstrate chaotic behavior under normal conditions. The system would, however resonate (or produce a single pattern more frequently) when it is presented with a pattern that it is trained with.
The network which we have investigated is the Adachi Neural Network (AdNN) [2–4], based on which we have, ourselves, developed results in various avenues [3–6], including that of designing a NN that can yield ideal chaotic PR [7]. In this paper we have considered how the topology can be modified so as to render the network to be much closer to “real” neural networks. To achieve this, we have changed the network structure to be that of a Small-world graph, and then computed the best weights for the new graph by using a gradient-based algorithm. Apart from a Lyapunov analysis, by a detailed experimental suite, we have shown that the new Smallworld-AdNN possesses chaotic and PR properties for different settings.

References

Detecting Chaos Using
the Strength of Extreme L Rule

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Abstract. For a time series we consider the quantity L, formally similar to angular
momentum, and strength of a rule, named the extreme L rule, about actual value
of L and two future time series elements. A four-dimensional vector is assigned to a
scalar time series by the numerical titration with low level noise. Mean strength of
the rule and standard deviation, for two levels of added noise, are the components of
this vector. It is shown that the values of Lyapunov exponent are close if vectors of
time series described by Feigenbaum map are close. Three sets of four-dimensional
vectors are formed – Rg, St and Ch, for artificial regular, stochastic and chaotic time
series respectively and their 2-norm distances are estimated. In such a manner we can
distinguish chaos with small noise from pure noise, including colored noise. Chaotic
time series are constructed using iterative maps (Feigenbaum, Henon, sine-square, ...
map) and three-dimensional ODEs (Lorenz, Ueda, Rikitake, ... equations). For an
experimental time series we find its four-dimensional vector and classify it, computing
2-norm distances to sets Rg, St and Ch. The proposed method is tested on a time
series measured in the experiment with RLC circuit. Our result is in agreement with
the results obtained by conventional methods.
Keywords: Time series, Chaos, Noise, Strength of rule, Numerical titration.

1 Introduction

In 2001 Poon and Barahona proposed a numerical titration procedure for de-
tection of chaos [8]. Their method is analogous to neutralization of the acid
with added base, for the purpose of determination of acid concentration. Poon
and Barahona add noise of increasing standard deviation to time series until
its nonlinearity goes undetected. Limiting value of standard deviation gives a
relative measure of chaos intensity.
Hu and Raman are confirmed chaotic nature of AFM tip oscillations by Lya-
punov exponent and noise titration calculations [3]. Chaotic human ventilation
was identified in the same manner [10]. Freitas, Letellier and Aguirre are found
that noise titration fails to distinguish colored noise from low-dimensional chaos
[2]. Roulin, Freitas and Letellier propose usage of this method for detecting a
nonlinear component in dynamics [9].

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The genuine Poon-Barahona method is not applied here, but the level of added noise is restricted on two low values. Noise affects the strength of a rule, we formulate using a quantity formally similar to angular momentum. Then we introduce four-dimensional vectors describing time series. Characterization of a measured time series is possible by comparison of two vectors – vector of measured time series and vector of an artificial time series of known character. Our goal is to avoid difficulties in computing entropies, dimensions and Lyapunov exponents of a measured time series [5].

2 Extreme L Rule

For a time series \( A_1, A_2, ..., A_{2000} \) we compute

\[
Z_k = (1 - b) \frac{A_k}{A_{max}} + bG_k
\]

where

\[
A_{max} = \max\{|A_k|; k = 1, 2, ..., 2000\}
\]

and \( G_k \) is Gaussian noise. In numerical titration procedure we will take two levels of noise: \( b = 10^{-6} \) and \( b = 10^{-3} \).

The quantity formally similar to angular momentum is

\[
L_j = X_jV_{yj} - Y_jV_{xj}, \quad j = 2, 3, ..., 999
\]

with

\[
V_{xi} = X_i - X_{i-1}, \quad V_{yi} = Y_i - Y_{i-1}
\]

and

\[
X_k = Z_{2k+1}, \quad Y_k = Z_{2k}
\]

We now formulate the extreme L rule. For \( N_\alpha \) (\( N_\beta \)) different values of \( m \)

\[
L_m > L_\alpha \quad (L_m < L_\beta) \quad \Rightarrow
\]

\[
\text{sign}(X_{m+1} - X_m) = \text{const.} \quad \text{and} \quad \text{sign}(Y_{m+1} - Y_m) = \text{const.}
\]

Strength of the rule is

\[
N_\alpha + N_\beta - 2
\]

For example, we take a time series with the following rule

\[
L_{80} > L_{400} > L_{300} > L_{658} > \cdots
\]

\[
L_{50} < L_{600} < L_{200} < L_{381} < \cdots
\]

\[
\text{sign}(X_{81} - X_{80}) = \text{sign}(X_{401} - X_{400}) = \text{sign}(X_{51} - X_{50}) = \text{sign}(X_{601} - X_{600}) = \text{sign}(X_{201} - X_{200}) = \text{sign}1
\]

\[
\text{sign}(Y_{81} - Y_{80}) = \text{sign}(Y_{401} - Y_{400}) = \text{sign}(Y_{51} - Y_{50}) = \text{sign}(Y_{601} - Y_{600}) = \text{sign}(Y_{201} - Y_{200}) = \text{sign}2
\]
where
\[
\text{sign}(X_{301} - X_{300}) \neq \text{sign}1 \quad \text{or} \quad \text{sign}(Y_{301} - Y_{300}) \neq \text{sign}2 \\
\text{sign}(X_{382} - X_{381}) \neq \text{sign}1 \quad \text{or} \quad \text{sign}(Y_{382} - Y_{381}) \neq \text{sign}2
\] (9)

Then
\[
L_\alpha = L_{300}, \quad L_\beta = L_{381}, \quad N_\alpha = 2, \quad N_\beta = 3, \quad N_\alpha + N_\beta - 2 = 3
\] (10)

The strength of extreme L rule in this case is three.

3 Four-Dimensional Vectors Assigned to Time Series

If level of noise in titration procedure is \( b = 10^{-6} \), we find strength of the rule \( S_1 \pm \delta S_1 \). If level of noise is \( b = 10^{-3} \), the strength of the rule is \( S_2 \pm \delta S_2 \). Then we construct four-dimensional vector
\[
< S_1, \delta S_1, S_2, \delta S_2 >
\] (11)

and assign it to considered scalar time series. In graphical representation of this vector, lengths of red, yellow, green and blue lines are equal to \( S_1, \delta S_1, S_2 \) and \( \delta S_2 \) (figure 1, figure 2).

Distance between two sets of four-dimensional vectors, \( \text{Set}_1 \) and \( \text{Set}_2 \), is
\[
d(\text{Set}_1, \text{Set}_2) = \text{min} \{|< P_{i1}, \delta P_{i1}, P_{i2}, \delta P_{i2} > - < Q_{j1}, \delta Q_{j1}, Q_{j2}, \delta Q_{j2} > |; \quad i = 1, 2, 3, ..., \quad j = 1, 2, 3, ... \}
\] (12)

where vectors \( < P_{i1}, \delta P_{i1}, P_{i2}, \delta P_{i2} > \) belong to \( \text{Set}_1 \), vectors \( < Q_{j1}, \delta Q_{j1}, Q_{j2}, \delta Q_{j2} > \) belong to \( \text{Set}_2 \) and \( || \) denotes 2-norm.

Considering damped oscillations
\[
Ce^{-\beta t} \sin \omega t, \quad t = 0.01k
\] (13)

we can see that values of \( \beta \) and values of \( \omega \) are close if corresponding four-dimensional vectors are close (figure 2). Therefore dynamics described by a time series and vector assigned to this time series are strongly connected.

For Feigenbaum map
\[
A_i = 1 - qA_{i-1}^2
\] (14)

values of the Lyapunov exponent
\[
\lambda = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \ln |2qA_{i-1}|
\] (15)

are approximately equal if vector components are approximately equal (figure 3).
We consider now time series $A_k = \xi(0.01k)$ constructed using Lorenz equations
\begin{align*}
\frac{d\xi}{dt} &= 10(\eta - \xi), \quad \frac{d\eta}{dt} = r\xi - \eta - \xi\zeta, \quad \frac{d\zeta}{dt} = \xi\eta - \frac{8}{3}\zeta \tag{16}
\end{align*}
with
\begin{align*}
\xi(0) = 9.4, \quad \eta(0) = 8.8, \quad \zeta(0) = -7.8 \tag{17}
\end{align*}
If vectors describing time series are close, then values of $r$ are close (figure 4).

In many cases we have considered, if two vectors $<P_1, \delta P_1, P_2, \delta P_2>$ and $<Q_1, \delta Q_1, Q_2, \delta Q_2>$ are close, namely
\begin{align*}
|| <P_1, \delta P_1, P_2, \delta P_2> - <Q_1, \delta Q_1, Q_2, \delta Q_2> || \\
<< || <P_1, \delta P_1, P_2, \delta P_2> ||, || <Q_1, \delta Q_1, Q_2, \delta Q_2> || \tag{18}
\end{align*}
then characters of corresponding time series are very similar. Reversed statement is not valid. If characters of two time series (type of chaos or type of regularity for example) are very similar, their vectors can be very different.

**Fig. 1.** First bundle contains vectors of eight stochastic time series. Lengths of red, yellow, green and blue lines are equal to $S_1, \delta S_1, S_2$ and $\delta S_2$. Eight vectors in the second bundle are assigned to eight regular time series (undamped periodic and quasi-periodic oscillations).
Fig. 2. Vectors of damped oscillations $Ce^{-\beta t} \sin \omega t$ ($t = 0.01k$), where (1) $\omega = 1$ and $\beta = 0.001 - 0.0011$ (first bundle), (2) $\omega = 1$ and $\beta = 0.003 - 0.0031$ (second bundle), (3) $\beta = 0.001$ and $\omega = 4.0 - 4.005$ (third bundle), (4) $\omega = 3.005 - 3.0051$ and $\beta = 0.002 - 0.0021$ (fourth bundle).

Fig. 3. Vectors of Feigenbaum map. Values of $\lambda$ are: (1) from -0.0203 to -0.0191 (first bundle), (2) from 0.4064 to 0.4093 (second bundle), (3) from 0.5399 to 0.5407 (third bundle), (4) from 0.6425 to 0.6457 (fourth bundle).
Fig. 4. Vectors of time series constructed using Lorenz equations. Four vectors in first bundle describe regular time series with $r = 10.2 - 10.4$. The following vectors describe chaotic time series with $r = 29.800002 - 29.800005$ (second bundle), $r = 30.100002 - 30.100005$ (third bundle), $r = 30.200002 - 30.200005$ (fourth bundle).

4 Sets of Vectors $Rg$, $St$ and $Ch$

We now form three sets ($Rg$, $St$ and $Ch$) containing four-dimensional vectors of artificial regular, stochastic and chaotic, with small noise, time series. Set $Rg$ contains vectors of regular time series (damped and undamped, periodic and quasi-periodic, oscillations and Feigenbaum map in regular regime). Form of the time series elements, in the case of undamped oscillations, is

$$A_k = \sum_i \left[ C_1 \cos \omega_i k + C_2 \cos(\Omega_i k + \phi_i) \right]$$ (19)

Vectors of stochastic time series there are in set $St$. We have generated random numbers with uniform and Gaussian distributions (white and colored noise). Colored noise in $St$ is generated by Bartosch algorithm [1].

Few hundred chaotic time series, described by vectors belonging to set $Ch$, are constructed using iterative maps (Feigenbaum, Henon, sine-square, etc) and three-dimensional ODEs (Lorenz, modified Lorenz, Rössler, Ueda, Rikitake, etc). The level of added noise in these time series is from zero to 0.01%. This noise is included in $A_j$. The noise included in $Z_k$ (eq. 1) is something else.
We analyze subseries the proper embedding dimension \[6\]. The mutual information is detected using basic methods – determinism test, attractor reconstruction and calculation of the largest Lyapunov exponent. The mutual information method and the false neighbor method yield the proper embedding delay and the proper embedding dimension \[6\].

### 5 Periodically Driven RLC Circuit

A time series \(K_i\) of length 25000 is measured in the experiment with periodically driven RLC circuit, performed by Kodba, Perc and Marhl \[7\]. \(K_i\) is the output voltage with a sampling rate of 500 measurements per second. Chaos is detected using basic methods – determinism test, attractor reconstruction and calculation of the largest Lyapunov exponent. The mutual information method and the false neighbor method yield the proper embedding delay and the proper embedding dimension \[6\].

We analyze subseries

\[A_i = K_{i+p} \quad (i = 1, 2, ..., 2000)\]  

and confirm presence of chaos (table 1).

<table>
<thead>
<tr>
<th>(p)</th>
<th>vector</th>
<th>(d(\text{vector}, Rg))</th>
<th>(d(\text{vector}, St))</th>
<th>(d(\text{vector}, Ch))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0 &lt; 1.0, 1.55, 0.88 &gt;</td>
<td>0.033</td>
<td>0.198</td>
<td>0.246</td>
</tr>
<tr>
<td>32</td>
<td>0 &lt; 1.0, 1.46, 0.96 &gt;</td>
<td>0.060</td>
<td>0.235</td>
<td>0.204</td>
</tr>
<tr>
<td>65</td>
<td>0 &lt; 0.0, 0.54, 0.73 &gt;</td>
<td>0.086</td>
<td>0.259</td>
<td>1.262</td>
</tr>
<tr>
<td>82</td>
<td>0 &lt; 1.0, 1.54, 1.03 &gt;</td>
<td>0.047</td>
<td>0.261</td>
<td>0.168</td>
</tr>
<tr>
<td>83</td>
<td>0 &lt; 0.0, 0.37, 0.60 &gt;</td>
<td>0.083</td>
<td>0.158</td>
<td>1.928</td>
</tr>
<tr>
<td>582</td>
<td>0 &lt; 0.0, 0.11, 0.31 &gt;</td>
<td>1.011</td>
<td>0.068</td>
<td>5.284</td>
</tr>
<tr>
<td>624</td>
<td>0 &lt; 0.0, 0.12, 0.33 &gt;</td>
<td>0.351</td>
<td>0.0</td>
<td>4.893</td>
</tr>
<tr>
<td>718</td>
<td>0 &lt; 0.0, 0.16, 0.37 &gt;</td>
<td>0.631</td>
<td>0.070</td>
<td>4.124</td>
</tr>
<tr>
<td>824</td>
<td>0 &lt; 0.0, 0.16, 0.39 &gt;</td>
<td>0.571</td>
<td>0.047</td>
<td>3.916</td>
</tr>
<tr>
<td>970</td>
<td>0 &lt; 0.0, 0.18, 0.39 &gt;</td>
<td>0.527</td>
<td>0.0</td>
<td>3.805</td>
</tr>
<tr>
<td>923</td>
<td>2 &lt; 2.0, 2.40, 1.39 &gt;</td>
<td>0.149</td>
<td>0.149</td>
<td>0.044</td>
</tr>
<tr>
<td>941</td>
<td>2 &lt; 2.0, 2.60, 1.46 &gt;</td>
<td>0.168</td>
<td>0.150</td>
<td>0.034</td>
</tr>
<tr>
<td>969</td>
<td>2 &lt; 2.0, 2.29, 1.49 &gt;</td>
<td>0.150</td>
<td>0.192</td>
<td>0.004</td>
</tr>
<tr>
<td>997</td>
<td>2 &lt; 2.0, 2.11, 1.04 &gt;</td>
<td>0.148</td>
<td>0.175</td>
<td>0.048</td>
</tr>
<tr>
<td>999</td>
<td>2 &lt; 2.0, 2.26, 1.19 &gt;</td>
<td>0.109</td>
<td>0.134</td>
<td>0.017</td>
</tr>
<tr>
<td>1001</td>
<td>2 &lt; 2.0, 2.21, 1.10 &gt;</td>
<td>0.098</td>
<td>0.135</td>
<td>0.016</td>
</tr>
</tbody>
</table>

**Table 1.** Considering time series measured by Kodba, Perc and Marhl we find regular subseries \((p = 0, 32, 65, 82, 83)\), stochastic subseries \((p = 582, 624, 718, 824, 970)\) and chaotic subseries \((p = 923, 941, 969, 997, 999, 1001)\).

### 6 Kobe Earthquake

We have computed vectors for subseries of the recorded Kobe earthquake time series \[4\]. Most often we find

\[d(\text{vector}, Rg) > 0, \quad d(\text{vector}, Ch) > 0, \quad d(\text{vector}, St) = 0\]  

\[22\]
with
\[ \text{vector} = <1, 0, 1, 0 > \text{ or } <2, 0, 2, 0 > \text{ or } <3, 0, 3, 0 > \]  \hspace{1cm} (23)

For other vectors, the distances often satisfy
\[ d(\text{vector}, \text{Ch}) > d(\text{vector}, \text{Rg}) \gg d(\text{vector}, \text{St}) > 0 \]  \hspace{1cm} (24)

and rarely much greater is replaced by greater
\[ d(\text{vector}, \text{Ch}) > d(\text{vector}, \text{Rg}) > d(\text{vector}, \text{St}) > 0 \]  \hspace{1cm} (25)

We can conclude that analyzed time series is stochastic one.

7 EEG Time Series

We consider here EEG time series \( E_k \) \((k = 1, 2, ..., 3595)\) recorded on a patient undergoing ECT therapy for clinical depression [11]. A vector is assigned to
\[ A_j = E_{j+p} \quad (j = 1, 2, ..., 2000; \ p = 1, 2, ..., 1595) \]  \hspace{1cm} (26)

with certain \( p \). Then we compute distance from the vector to sets \( \text{Rg}, \text{St} \) and \( \text{Ch} \). When \( p \) is increasing, the vector oscillates between \( \text{St} \) and \( \text{Ch} \), or between \( \text{Rg} \) and \( \text{Ch} \) (table 2).

<table>
<thead>
<tr>
<th>( p )</th>
<th>( \text{vector} )</th>
<th>( d(\text{vector}, \text{Rg}) )</th>
<th>( d(\text{vector}, \text{St}) )</th>
<th>( d(\text{vector}, \text{Ch}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( &lt;1, 0, 1.27, 1.54 &gt; )</td>
<td>0.27</td>
<td>0.38</td>
<td>0.06</td>
</tr>
<tr>
<td>2</td>
<td>( &lt;13, 0, 13.15, 0.39 &gt; )</td>
<td>0.07</td>
<td>0.02</td>
<td>0.43</td>
</tr>
<tr>
<td>3</td>
<td>( &lt;1, 0, 1.53, 2.12 &gt; )</td>
<td>0.31</td>
<td>0.37</td>
<td>0.02</td>
</tr>
<tr>
<td>4</td>
<td>( &lt;13, 0, 13.07, 0.33 &gt; )</td>
<td>0.07</td>
<td>0.02</td>
<td>0.42</td>
</tr>
<tr>
<td>5</td>
<td>( &lt;1, 0, 1.17, 1.20 &gt; )</td>
<td>0.09</td>
<td>0.38</td>
<td>0.06</td>
</tr>
<tr>
<td>6</td>
<td>( &lt;13, 0, 13.13, 0.34 &gt; )</td>
<td>0.07</td>
<td>0.02</td>
<td>0.43</td>
</tr>
<tr>
<td>7</td>
<td>( &lt;1, 0, 1.15, 2.19 &gt; )</td>
<td>0.33</td>
<td>0.37</td>
<td>0.04</td>
</tr>
<tr>
<td>8</td>
<td>( &lt;13, 0, 13.13, 0.34 &gt; )</td>
<td>0.07</td>
<td>0.02</td>
<td>0.43</td>
</tr>
<tr>
<td>751</td>
<td>( &lt;1, 0, 1.40, 1.97 &gt; )</td>
<td>0.27</td>
<td>0.38</td>
<td>0.08</td>
</tr>
<tr>
<td>752</td>
<td>( &lt;17, 0, 17.03, 0.17 &gt; )</td>
<td>0.08</td>
<td>0.12</td>
<td>0.55</td>
</tr>
<tr>
<td>753</td>
<td>( &lt;1, 0, 1.77, 2.63 &gt; )</td>
<td>0.43</td>
<td>0.39</td>
<td>0.18</td>
</tr>
<tr>
<td>754</td>
<td>( &lt;17, 0, 17.01, 0.10 &gt; )</td>
<td>0.08</td>
<td>0.12</td>
<td>0.55</td>
</tr>
<tr>
<td>755</td>
<td>( &lt;1, 0, 1.60, 2.39 &gt; )</td>
<td>0.38</td>
<td>0.38</td>
<td>0.11</td>
</tr>
<tr>
<td>756</td>
<td>( &lt;17, 0, 17.01, 0.10 &gt; )</td>
<td>0.08</td>
<td>0.12</td>
<td>0.55</td>
</tr>
<tr>
<td>757</td>
<td>( &lt;1, 0, 1.39, 1.92 &gt; )</td>
<td>0.26</td>
<td>0.39</td>
<td>0.09</td>
</tr>
<tr>
<td>758</td>
<td>( &lt;17, 0, 17.0 &gt; )</td>
<td>0.09</td>
<td>0.12</td>
<td>0.55</td>
</tr>
</tbody>
</table>

**Table 2.** Results we are obtained investigating subseries of EEG time series. For \( p \) from 1 to 8, the vector approaches to \( \text{Ch} \), then to \( \text{St} \), again to \( \text{Ch} \), and so on. For \( p \) from 751 to 758 similar oscillations happen, but \( \text{St} \) is replaced by \( \text{Rg} \).
8 Conclusion

A new method for time series analysis is proposed here. The extreme L rule and four-dimensional vectors assigned to time series are in the basis of this method. In plenty of examples, closeness of vectors leads to similar characters of time series described by these vectors. We compute distances from vector of a measured time series to sets \( R_g \), \( St \) and \( Ch \), containing vectors of artificial regular, stochastic and chaotic time series. If minimal distance is significantly smaller than other distances, we assume that the character of time series is determined correctly with high probability.

In our further investigations we can add vectors of other artificial time series to sets \( R_g \), \( St \) and \( Ch \). It is also possible to replace \( Ch \) with a few sets corresponding to different types of chaos.

References

Simulation of Grain Structures on Steel Billets Solidified During Continuous Casting.


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Abstract: During continuous casting process (CCP), liquid steel is cast from the tundish to a mold. Here the steel adopts the mold section geometry (squared section) and begins to be quenched using a primary cooling system incorporated in the mold walls. Then steel billets are quenched using a secondary cooling system. Finally the steel billets are driven along a free zone to be cut and stored as a new product. During this industrial process, different grain structures are formed as a function of the heat removal conditions and the corresponding solidification speed. Near the billet surfaces a chill zone is initially formed followed by a columnar grain zone and finally an equiaxed zone in the core. A computational simulator based on stochastic methods and cellular automaton (chaos theory) is described in this work. The algorithms and equations used are also explained in detail. Computational arrays of the heat removal process previously calculated are saved and reloaded to assign solidification times and rebuild the billet thermal history [5]. The simulator includes computational algorithms for grain nucleation and grain growth in every zone. Routines for pre-nucleation and pre-growth have been also added for an improved simulation and a graphical user interface was used to display on the screen the structures simulated.

Keywords: Grain structures (Chill, columnar and equiaxed grains), Steel billets, chaotic morphology, metals Solidification.

1. Introduction.

Simulation of grain structure formation during steel solidification is a complex process. Many computational algorithms have been developed by many authors [1-26]. Some of them have been working on the solution of the heat removal conditions during the CCP [1-4]. The first mathematical models were based on interpolation methods to predict the steel thermal behavior due to the limits on computational data processing speed and limited storage capacity. Nevertheless some researchers [2-3] continued developing more efficient programs and models according with the increment on computing capacities. Others [4-7] have been using new finite element software packages capable to solve heat and mass transfer equations. Some others have studied anisotropy of the material properties and related with the new mathematical theories such as stochastic, probabilistic and statistical methods;
which were developed to describe the particular complex geometries in the nature such as cellular automaton and fractals [5-26]. Many of these theories are based on the management of statistical information of analyzed samples such as grain size and grain population. Then a computational algorithm is programmed to establish a relationship with a random process. The Monte Carlo and cellular automaton [6-11 & 19-23] are two of the most popular methods used for simulation due to these can be easily programmed using random instructions to be included in calculation routines. The Monte Carlo Method is based on the computational generation of random numbers. This method has been widely used in material science to develop 2D and 3D computational models for representing heterogeneity on materials properties and sophisticated morphologies of solids [5-26]. Some authors have been working on mathematical models for the solidification of metals and alloys using heterogeneous distributions of metals and phases [6-12 & 19]. Some authors dedicated emphasis in dendritical growth [14-18]. Crystal and grain growth have been studied as a function of the dwell time on liquid, mushy and final solidification [9]. Other authors have been developed models to calculate the geometrical transformation during recrystallization [10-12]. The cellular automaton theory has also been used to create models for phase transformations and simulate microstructures of grains for different metallic materials [6-11 &19-23]. Other researchers have been analyzed the influence of simulation scales (micro, meso & macro) [13 & 18] for simulating microstructures and nano-structures. Other authors have studied the influence of the processing methods over physical and chemical properties of materials. These new mathematical theories have been developed in the last three decades becoming very popular establishing the computational relationships between deterministic and stochastic processes. The Model developed in the present work to simulate the different grain structures in a steel billet solidified, uses computational algorithms to reproduce grain nucleation and growth processes. Heat removal conditions and particular nodal solidification speed are compared with pre-defined values to establish the boundary between different grain sizes and morphologies formed and reproduce the grain growth.

2. Reading and management of the information.

The steel was discretized using a regular squared mesh and solved using a finite difference method to calculate the thermal behavior in a previous work [5]. Steel was considered as homogeneous and every node in the mesh represented the same energy (H_{ij}) to foundry a steel volume until the casting temperature (initial temperature). When the steel is cast; the energy and temperature on every node decrease due to heat removal conditions. The steel originally in a liquid state is quenched to mushy and then to a final solid state. The simulator developed by the present authors [5] calculates the steel thermal behavior as a function of many factors such steel composition, casting speed, and the operating conditions. Then solidification and temperature profiles were displayed on the screen using nested
loops routines. These loops were profited for including in the main thermal solution a routine to save the calculated information at each step time. Temperature in each node of the steel discretized is calculated as a function of the corresponding heat latent \( T_{\text{I,J}} = f(H_{\text{I,J}}) \) and the heat removal conditions \( -q_{\text{I,J}} \) applied after each iteration. These temperatures are compared with the changing state temperatures \( T_{\text{liq}} \) and \( T_{\text{sol}} \). When both values are identical the corresponding simulation times are stored in two independent 2D computational arrays to be saved in two independent files at the end of the simulation. The times \( t_{\text{I,J}} \) are declared as floating point data type for a more precise calculation. The saved times are ordered as \( (t_{\text{liq},\text{I,J}} \& t_{\text{sol},\text{I,J}}) \) to be identified and read using the new grain growth model developed. Moreover the information about the billet geometry and dimensions, the step time \( (\Delta t) \) and casting conditions such as the casting temperature \( T_c \), the casting speed \( c_s \), etc. are stored using a code number used to recognize the every factor involved during casting. This information is read independently by the grain growth simulator; which makes possible to create a grain structure without repeating the calculation of the steel thermal behavior. The 2D computational arrays are recognized reading the additional information firstly to establish the upper limits \( (nx) \) and \( (ny) \) to be used for the nested loops which commands the simulation process. The read values are loaded and stored in two new restored computational arrays; a numeric encoding is used to identify these values; number (1) is used for \( "T_{\text{liq}}" \) and (2) is for \( "T_{\text{sol}}" \) respectively. Here the main loop for the simulation process goes from an initial time \( (t=0) \) to the final solidification time registered \( (t_{\text{max}}) \). The main loop uses the previously saved step time \( (\Delta t) \) to command the simulation; and the saved nodal times \( (t_{\text{liq},\text{I,J}} \& t_{\text{sol},\text{I,J}}) \) are compared with the simulation time \( (t+\Delta t) \) using a single identification routine to rebuild the steel thermal history placing the nodes on the screen. The mushy time is obtained using equation (1). Moreover it is possible to calculate the fraction of solid \( (X_{\text{sol},\text{I,J}}) \) and liquid \( (X_{\text{liq},\text{I,J}}) \) simultaneously using equations (2) and (3) respectively due to the time representation is analogous to the temperature and to the solid fraction. This calculation permits the node be classified as a function of its actual solidification status.

\[
\begin{align*}
    t_{\text{mushy},\text{I,J}} & = (t_{\text{liq},\text{I,J}} - t_{\text{sol},\text{I,J}}) \\
    X_{\text{sol},\text{I,J}}^t & = \frac{t - t_{\text{sol},\text{I,J}}}{t_{\text{sol},\text{I,J}} - t_{\text{liq},\text{I,J}}} \\
    X_{\text{liq},\text{I,J}}^t & = 1 - X_{\text{sol},\text{I,J}}^t
\end{align*}
\]

The algorithm shown in the flow chart shown of figure (1) is used to count the solidified nodes and display a solidification profile on the screen as is shown in figure (2). Here the variables \( (n\text{l}^t), (n\text{m}^t) \) and \( (n\text{s}^t) \) count the nodes on liquid, mushy
and solid respectively; these are initialized equal to zero to begin every new counting process at each step time \(t + \Delta t\). At the end of the loops execution these variables are stored to display the solidification speed graphs shown in figures (3, 4 & 5). Solidification begins inside the mold. Here liquid steel is quickly quenched on the billet surfaces. In consequence a lot of nodes change from liquid to solid state instantly; and the mushy time is very short. Nevertheless the solidification speed decreases and mushy time becomes longer. Figure (3) shows an accounting of the total nodes that goes from liquid to mushy and from mushy to solid during simulation. These graphs are cumulative. The vertical slopes in both curves at the beginning evidence a high solidification speed. Horizontal slopes at the ending indicate the reduction of the solidification speed. The region between these two curves is the mushy time. The last node on changing to mushy was at 74s. Which makes match with the longest mushy time with the maximum nodes on mushy registered on figure (4). The slope in this graph also is vertical at the beginning of the solidification, confirming a high solidification speed. The chill zone is formed here. After that the slope becomes to decrease and the columnar grain zone grows and finally the equiaxed grains begin to appear when the mushy time becomes very long. Nevertheless the solidification speed is reduced suddenly after 10s. Although the nodes changing state continue being increased due to the heat latent inside the billet section. Finally after (74s.) the number is decreased due the absence of liquid steel. The instantaneous changing state speeds are shown in figure (5). In the same way than the other graphs here a lot changing state nodes were registered at the beginning of the solidification until reach a maximum value confirming a high solidification speed. Then both are reduced due to the nodes changing state are slowly decreased.

Figure (1). Flow chart for counting the nodes on liquid, mushy and solid.  
Figure (2). Solidification profile.
3. Nucleation, Growth, Pre-nucleation and Pre-growth.

Steel solidification is a complex problem and different grain structures are formed according with the solidification speed. The most common procedures involves during solidification are Nucleation and growth. Nucleation happens when the simulation time is greater or equal than the individual node solidification time ($t > t_{sol I,J}$). Nucleation is an independent process for each node. A nodal nucleation is accepted after a positive identification in the comparison between a local probability of nucleation and a random number generated as is done in Monte Carlo method. If this second identification is true a new grain is born. Then a new random number is generated in order to assign a color and then the corresponding pixel is printed on the screen coordinates. In contrast growth process is a dependent process. If the condition ($t > t_{sol I,J}$) is true but the second identification is negative the node will be considered as available to be growth with a solidified neighbor using a searching routine. In that way, all the solidified neighbors surrounding the pivoting node are considered for growing with. A probability corresponding with their proximity and solidification time is assigned; and the Monte Carlo Method is used to select randomly the neighbor for growing with. Then the color of the neighbor selected is assigned to the pivoting node. Additionally procedures such as pre-nucleation and pre-growth are included in the algorithm to obtain a better approach. These are included to represent the probability that a pivoting node can be solidified before its
solid fraction reach the unit ($X_{sol,I,J}<=1$). The routines developed for nucleation and growth process are used for solving these procedures in order to avoid unnecessary code and make more efficient the algorithm. Nevertheless the searching routines are modified according to the grain structure to be formed. Each node will be a part of only one single grain during simulation; reason why the algorithm takes in counts the following assumptions:

A pivoting node is the node which is being analyzed.

The mushy time ($t_{mushy,I,J}$) is used to identify the grain zone by comparison.

A node is solidified only one time when the sentence ($t>t_{sol,I,J}$) is true.

A node is only change to be pre-nucleated according with its solid fraction.

A pre-solidified node is registered as a solidified node.

A pre-growth node is registered as a solidified node.


The flow chart shown in figure (6) explains the process for identification of the grain zones. The first grain structure formed during steel solidification is well known as chill zone. A high solidification speed forms quickly a shell thickness formed with a great number of little size equiaxed grains are formed in this zone as a consequence of the high solidification speed. Here grain nucleation is the most frequent solidification procedure; grain growth is limited due to the simultaneous growth of many neighboring nucleated grains. At the beginning of solidification the mushy time is very short, in consequence its calculation is also considered as not necessary. In the same way pre-nucleation and pre-growth routines are not included for being considered as not needed during the formation of the chill zone. The boundary for the formation of the chill zone is ($t_{chill}=2.0s$). This value is compared with the mushy time and if the sentence ($t_{mushy,I,J}<=t_{chill}$) is true the algorithm is employed. Solidification speed decreases as the times goes due to the shell thickness formed reduces the heat removal capacity and the nodes inside the billet remain longer times on liquid and mushy. If the sentences ($t_{mushy,I,J}>t_{chill}$) and ($t_{mushy,I,J}<t_{col}$) are true; the algorithm for columnar zone is employed. Here the growth process will be the most frequent process. Nucleation of new grains rarely happens in columnar and equiaxed zones. Nevertheless in both these zones, pre-nucleation and pre-growth of new grains are commonly occurring. The boundary for the formation of the columnar zone is ($t_{col}=12.5s$). Finally if the sentence ($t_{mushy,I,J}>t_{col}$) is true the algorithm for the equiaxed zone is applied.

The inclusion of pre-nucleation and pre-growth procedures generates new grains ($n_{npq}$) which must be counted in order to know the number of available un-solidified nodes ($n_{ng}$) at each solidification time ($t+\Delta t$) during the simulation. When the sum ($n_{npq}+n_{ng}$) is equal to total solidified nodes at that time ($n_{tot,sol}$) the loop is break
and the values are returned to initial values and the entire process begins for the next step time. Here the each new solidified node is counted after the pre-nucleation and pre-growth routines have been executed and before nucleation and growth procedures were executed as is shown in the shaded area of figure (6). This routine is compiled separately and nested to be employed in the columnar and equiaxed zones. Pre-growth and growth are randomly selective procedures that involve a particular neighboring analysis about the pivoting node in order to transform the numerical information of the thermal analysis in a cellular automaton. A cellular automaton is a computational algorithm for describing spatial and temporal evolution of complex system by applying local or global stochastic and deterministic transformation rules. The evolution of the cellular automata takes place through the application of the transformation rules that act on the state of each node and determine the state of a node as a function of its previous state or the state of the neighboring nodes. Then the new state of the variables used is updated simultaneously for all nodes. The value of an arbitrary state variable \( \xi \) assigned to a particular node at a time \((t + \Delta t)\) is a function of its present state and the state of its neighbors. The equation (4) shows formally this relation for a two dimensional analysis considering the 4 nearest neighbors. This is well known as von Newman neighboring. Nevertheless the equation (5) is also widely used due to the inclusion of the 4 next nearest neighbors is necessary in many analysis. This is called Moore neighboring.

\[
\xi_{i,j}^{t+\Delta t} = \left( \xi_{i-1,j}^t, \xi_{i+1,j}^t, \xi_{i,j-1}^t, \xi_{i,j+1}^t \right) \\
\xi_{i,j}^{t+\Delta t} = \left( \xi_{i-1,j-1}^t, \xi_{i-1,j+1}^t, \xi_{i+1,j-1}^t, \xi_{i+1,j+1}^t, \xi_{i-1,j}^t, \xi_{i+1,j}^t, \xi_{i,j-1}^t, \xi_{i,j+1}^t \right) 
\]

In columnar zone different preferential growth directions are adopted by the grains. Here grains are growth from the chill zone boundary towards the billet centre against the heat flux direction. In this zone preferential growth directions are calculated for each pivoting node using two-dimensional von Newman configurations considering the 4 nearest neighbors as is shown in figure (7a). The first step is to search the solidified neighbors. Equal probabilities are assigned to the nodes beside the pivoting node. Nodes in front are hotter than the pivoting node and frequently un-solidified; reason why the probabilities assigned to them are minor. In contrast nodes behind the pivoting node (those nearest to the billet surface) frequently are solidified reason why the major probability for growing is assigned to them. Nevertheless these assumptions can be improved in order to give a preferential probability for growing; calculating the distances from the pivoting node to the 4 billet surfaces using the equations (6-9). These distances are sum and the probabilities \( P_{b,i} \) are assigned to the neighbors according from the nearest to the fares surface using the equation (10). The general algorithm is shown is figure (8).
During growth, the pivoting node is compared to be identified as un-solidified node and the previously solidified neighbors are searched. Nevertheless these conditions are inverted for pre-growth. Here the pivoting node is compared to be identified as a pre-nucleated node and the un-solidified neighbors are searched. In consequence the searching criterion is inverted as is shown in figure (7b) for the von Newman neighboring. If the condition for pre-growing node is true; the pivoting node will
grow towards a billet surface in the same direction than the heat flux. Nodes in equiaxed zone remain a long time in mushy and their solidification speed is very slow. The hypothesis here is that pre-nucleation, pre-growth and growth are also frequent procedures. Nevertheless preferential growth directions are calculated for each pivoting node using two-dimensional Moore configurations considering the 8 nearest neighbors as is shown in figures (9a) and (9b). Here the difference in time between the pivoting node and the neighbors is calculated in order to find the shortest. A pair of loops including this procedure is nested in order to avoid unnecessary code. The differences are calculated using the equation (11) where the sub indexes “i” and “j” are used to identify each neighbor. Due to the 4 nearest neighbors indicated in the von Newman are nearer than those in the Moore neighboring a correction according with their distance to the pivoting node must be applied solving the equation (12) for every neighbor. Then the preferential probabilities are assigned according with the shortest difference time. Here a sentence “if” is also included in the searching routines in order to eliminate an unavailable neighbor at every time.

\[ d_{i,j} = t_{\text{solid},j} - t_{i,j} \]  

(11)

\[ d_{i,j} = \sqrt{(1-i)^2 + (J-j)^2} \]  

(12)

Figure (8). Flow chart for searching neighbors analysis.

Figure (9). Routines for two-dimensional searching nodes during growth and pre-growth with Moore neighboring.
Some assumptions for the equiaxed zone are the following:

A node is considered as available to be pre-nucleated or pre-growth if the sentence \((X_{s,t,L})\geq 0.5\) is true. Although the probability is increased as the solid fraction is also increased.

A preferential probability for growing is assigned to a neighbor as a function of the shortest time deference in the equiaxed zone; nevertheless similar results can be obtained if the probabilities are assigned as a function of the neighbor’s solid fraction.

5. Simulations.
The solidification times were obtained after calculate the steel thermal behavior of a squared steel billet (160 x 160 mm.) using the operating conditions shown in table (1). Here \((\Omega)\) is the shooting angle and \((d_{bs})\) is the distance (billet surface to spray) for the secondary cooling system (SCS).

The continuous casting machine is symmetrical and the same operating conditions were applied over the 4 billet surfaces. The radius on the curved zone is \((r_c=9.0\ \text{m})\), the casting speed was \((2.35\ \text{m/min})\) and the casting temperature was \((1524\ \text{C})\). Figure (10) shows a \(1/4\) cut of a steel billet. Here is shown the location of the 3 grain zones. Figure (11) is an example of the grain structures obtained using the model developed. Here the cellular automaton forms a digital image displayed on the screen. The grain size and grain orientation according with the corresponding grain zone and the each node position are appreciated in detail.

<table>
<thead>
<tr>
<th>Information</th>
<th>1</th>
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<th>3</th>
<th>4</th>
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<tbody>
<tr>
<td>Water flow rate</td>
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<td>195</td>
</tr>
<tr>
<td>Sprays</td>
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<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>(\theta)</td>
<td>2</td>
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<td>16</td>
</tr>
<tr>
<td>(\Omega)</td>
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<td>60</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>(d_{bs}) (mm)</td>
<td>160</td>
<td>160</td>
<td>160</td>
<td>160</td>
</tr>
</tbody>
</table>
6. Conclusions.
After the execution of the algorithms and the simulation of the solidification process it is possible confirms:

At the beginning a high solidification speed, corresponds to a short mushy time. In consequence a lot of nodes are quickly nucleated forming a zone with little equiaxed grains.

The growth orientation depends of the heat flux direction. Evidence is appreciated in the columnar zone.

The structures obtained confirmed the strong influence of the solidification speed and mushy time [9] over the grain structure to be formed as is shown in figure (11). Here the grain size becomes bigger as the simulation time goes and as the mushy time becomes longer.

The model developed in the present works is capable to reproduce in detail the grain structures (chill, columnar and equiaxed) formed during the solidification of a steel billet.

Acknowledgments
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References.

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The Ni-Al-Zr diffusion simulations

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Abstract: In this paper the bi-velocity is applied to calculate the behavior of high zirconium content alloys in the Ni-Al-Zr system. The method allows a quantitative description of diffusion mass transport in multi-phase materials. The method links the bi-velocity Darken approach with the phase-field model in which the diffusion zone is quantitatively characterized by phase volume fractions. The chemical potentials of components in the ternary Ni-Al-Zr system are predicted numerically on the basis of thermodynamic properties of binary systems included in the investigated ternary system. The idea of predicting $\text{ijk}^\text{ex}G$ values is regarded as calculation of values of $\text{ex}G$ function inside a certain area (a Gibbs triangle) unless all boundary conditions, that is values of $\text{ij}^\text{ex}G$ on all legs of the triangle are known ($\text{ij}^\text{ex}G$, $\text{ik}^\text{ex}G$, $\text{jk}^\text{ex}G$). This approach is contrary to finding a function value outside a certain area, if the function value inside this area is known. The results of the calculations are compared with experimental concentration’s profiles of nickel, zirconium and aluminum in zirconium doped aluminide coatings deposited on pure nickel by the PVD and CVD methods.

Keywords: NiAlZr system, reactive diffusion, simulation, Zr content

1. Introduction.

The aluminizing process is extensively used to form protective coatings on aircraft turbine blades made of superalloys [1]. Aluminizing process is realized in many ways, such as: pack cementation, above-the-pack or physical and chemical vapor deposition methods. Addition of small amounts of reactive elements such as Zr, Hf, Y, or Ce to NiAl coatings has beneficial effects on the oxidation behavior. This beneficial effects include improvement of adhesion of alumina scales and reduction of oxide scale growth rate [2-6].

The problem of designing the technology of coatings’ deposition by CVD and PVD methods and designing the layers formed during aluminization remains open. The main difficulty is included in description of diffusion in a multi-component solid which leads to multi layers formation.

In this work, the bi-velocity method is generalized and combined with the phase field model. The fusion of these two methods, referred as the Bi-velocity Phase Field Method, is applied to calculate composition–distribution profiles for elements present in the diffusion couple. Hence, the diffusion path, which in the ternary phase diagram connects the terminal composition of the diffusion couple can be calculated. When the isothermal section of the phase diagram is projected onto the composition triangle, then the fields crossed by the diffusion path can be indicated. In this work the Ni-Al-Zr system is analyzed. The previous binary [7,8] model is expanded and mass transport in the
multicomponent system is taken into account, in which the layers of various phases and
multiphase layers can grow. The previous model is generalized and combined with the
phase-field approach. Values of chemical potentials of aluminum nickel and zirconium in
ternary Ai-Ni-Zr alloys were predicted numerically on the basis of thermodynamic
properties of binary systems included in the investigated ternary system.

2. The Model and Simulations
The interdiffusion may be described by means the generalized Darken or Onsager analysis
[9]. In this paper the Darken method coupled with the Phase Field Method [10,11] is used.
The core of the generalized Darken method is the mass conservation law:

$$\frac{\partial \bar{c}_i}{\partial t} + \text{div} \left( \bar{c}_i \bar{D}^d_i + \bar{D}^{drift}_i \right) = 0$$

(1)

where $\bar{c}_i$ denotes the average concentration of the i-th component in the j-th phase; $\bar{D}^d_i$ and $\bar{D}^{drift}_i$ are the average diffusion component velocity and the overall drift velocity, respectively.

In the presented analysis, a motion of a single phase $r$-component mixture, i.e., alloy or
solid solution is taken into account. The molar ratio, $N_{i,j}$ is defined as:

$$1 := \sum_i N_{i,j} := \sum_i \frac{c_{i,j}}{\bar{c}_j}$$

(2)

The mixture molar concentration in the j-th phase is a sum of the components molar
concentrations and for simplification is accepted constant:

$$\sum_i c_{i,j} = c_j = \text{const.}$$

(3)

The component diffusion velocity, $\bar{v}^d_{i,j}$, should be expressed by the proper constitutive
formula. In this work the Nernst-Planck equation is implemented:

$$\bar{v}^d_{i,j} = -B_{i,j} \frac{\partial \mu^{ch}_{i,j}}{\partial x},$$

(4)

where $\mu^{ch}_{i,j}$ is the chemical diffusion potential of the i-th component in the j-th phase; $B_{i,j}$
denotes the mobility.

The chemical potential can be expressed by the molar concentration as:

$$\mu^{ch}_{i,j} = \mu^{0}_{i,j} + RT \ln \left( c_{i,j} \gamma_{i,j} \right),$$

(5)

where $\mu^{0}_{i,j}$ denotes the standard, constant chemical potential of the i-th component and
$\gamma_{i,j}$ its activity coefficient.

Finally, by coupling Eqs. 4 and 5, the diffusion velocity of the components can be
expressed as:
\[ u_{i,j} = -RTB_{i,j} \frac{\partial \ln c_{i,j}}{\partial x}. \] (6)

The drift velocity can be calculated from the mass conservation of the components, with additional assumption of constant total molar concentration, thus:

\[ 0 = \sum_i \frac{\partial c_{i,j}}{\partial t} = \sum_i \frac{\partial}{\partial x} \left( c_{i,j} u_{i,j}^d + c_{i,j} u_{i,j}^{\text{drift}} \right) \] (7)

finally, the drift velocity equals:

\[ u_{i,j}^{\text{drift}} = -\sum_i \frac{c_{i,j}}{c_j} u_{i,j}^d. \] (8)

The average composition of the system in the spatial region is a weighted average of the compositions of the phases in the equilibrium, i.e. the compositions described by the tie-line ends, Fig. 1. The mass balance expressed for each component says:

\[ \bar{c}_i = f_{\alpha} c_{i,\alpha} + (1-f_{\alpha}) c_{i,\beta}, \quad i = 1, 2, 3. \] (9)

In the one-phase region there is simply:

\[ \bar{c}_i = c_{i,\alpha} \text{ or } \bar{c}_i = c_{i,\beta} \] (10)

depending on the phase.

The volume fraction, \( f_j \), in a two-phase region, \( c_{i,j} \) and \( \nu_{i,j} \) are the concentration and overall velocity of the \( i \)-th component in \( j \)-th phase,

\[ f_{\alpha} + f_{\beta} = 1, \quad 0 \leq f_j \leq 1. \] (11)

Finally, the mass conservation in single \( \alpha \) and \( \beta \) phase regions can be rewritten in a form:

\[ \frac{\partial f_j c_{i,j}}{\partial t} + \text{div} \left( f_j c_{i,j} \nu_{i,j} \right) = 0, \quad i = 1, 2, 3, \quad j = \alpha, \beta \] (12)

The overall average flux of the \( i \)-th component can be defined as:

\[ \bar{\nu}_i = -f_{\alpha} D_{i,\alpha} \frac{\partial c_{i,\alpha}}{\partial x} - f_{\beta} D_{i,\beta} \frac{\partial c_{i,\beta}}{\partial x} + f_{\alpha} c_{i,\alpha} \nu_{i,\alpha}^{\text{drift}} + f_{\beta} c_{i,\beta} \nu_{i,\beta}^{\text{drift}}, \quad i = 1, 2, 3 \] (13)

Figure 1 present the schematic presentation of the proposed method - the interdiffusion of the three component system between \( \alpha \) and \( \beta \) phases. On the composition triangle the phase boundaries are presented (functions \( g_{\alpha} \) and \( g_{\beta} \)). Lines connecting boundaries show the tie-lines (conodes), which are the initial conditions from the phase diagram.
Values of chemical potentials $\mu_i^\text{ch}$ (equation 4) of aluminum, nickel and zirconium were calculated on the basis of thermodynamic properties of binary systems included in the investigated ternary system. The idea of predicting $\Delta G_{ijk}$ values is regarded as calculation of values of $\Delta G$ function inside a certain area (a Gibbs triangle) unless all boundary conditions, that is values of $\Delta G$ on all sides of the triangle, are known ($\Delta G_{ij}$, $\Delta G_{ik}$, $\Delta G_{jk}$). This approach is contrary to finding a function value outside a certain area, if the function value inside this area is known (this issue is well known in mathematics). In this approach, values of excess Gibbs functions for all concentrations of binary alloys are taken into consideration, not only the selected ones and there is no problem with choosing binary mole fractions and proper weighting, unlike in geometrical models. In this approach, weighting of each mole fraction is the same. This model was successfully applied to Cu-Sn-Zn and Bi-Cu-Ni alloys [12] and results agree very well with the values obtained by the Calphad method.

The excess Gibbs energy $\Delta G$ describes the influence of non-ideal mixing behavior on the thermodynamic properties of a solution phase. The Muggianu [13] extension of the Redlich-Kister formalism [14] is a widely accepted description of the excess Gibbs energy:

\[
\Delta G = x_i x_j \sum_{z=0}^{m} z L_{ij} (x_i - x_j)^z + x_i x_k \sum_{z=0}^{m} z L_{ik} (x_i - x_k)^z + x_j x_k \sum_{z=0}^{m} z L_{jk} (x_j - x_k)^z \quad \text{for} \quad z = 0, 1, \ldots, m, \quad (14)
\]
where $L_{ij}$ are binary and $L_{ijk}$ is ternary temperature dependent interaction parameters optimized on the basis of the available thermodynamic and phase diagram data.

$$L_{ijk} = x_i^0 L_{ijk} + x_j^1 L_{ijk} + x_k^2 L_{ijk}$$  \hspace{1cm} (15)

Thermodynamic parameters for binary alloys were accepted from Huang and Chang [15] for Al-Ni, Wang et al. [16] for Al-Zr and Wang et al. [17] for Ni-Zr.

$$L_{\text{Al,Ni}} = -168292 + 16T + 32712 \cdot (x_{\text{Al}} - x_{\text{Ni}}) + (7998 + 35T) \cdot (x_{\text{Al}} - x_{\text{Ni}})^2$$  \hspace{1cm} (16)

$$L_{\text{Al,Zr}} = -165348 + 13.235T - 36570 \cdot (x_{\text{Al}} - x_{\text{Zr}}) + 16806 \cdot (x_{\text{Al}} - x_{\text{Zr}})^2$$  \hspace{1cm} (17)

$$L_{\text{Ni,Zr}} = -125000 + 5.25T$$  \hspace{1cm} (18)

As a result of calculations the following values of ternary $L$ parameters for 1273K were obtained:

$$L_{\text{Al,Ni,Zr}} = -1.3 \cdot 10^7 x_{\text{Al}} + 3.3 \cdot 10^6 x_{\text{Ni}} - 5 \cdot 10^6 x_{\text{Zr}}$$  \hspace{1cm} (19)

Values of chemical potentials of aluminum and zirconium were derived from excess Gibbs energy according to the following formulas:

$$\mu_{\text{Ni}} = \mu_{\text{ex}}^{\text{AlNiZr}} + (1 - X_{\text{Ni}}) \frac{\partial \mu_{\text{ex}}^{\text{AlNiZr}}}{\partial X_{\text{Ni}}} - X_{\text{Zr}} \frac{\partial \mu_{\text{ex}}^{\text{AlNiZr}}}{\partial X_{\text{Zr}}}$$  \hspace{1cm} (20)

$$\mu_{\text{Al}} = \mu_{\text{ex}}^{\text{AlINiZr}} - X_{\text{Ni}} \frac{\partial \mu_{\text{ex}}^{\text{AlINiZr}}}{\partial X_{\text{Ni}}} - X_{\text{Zr}} \frac{\partial \mu_{\text{ex}}^{\text{AlINiZr}}}{\partial X_{\text{Zr}}}$$  \hspace{1cm} (21)

$$\mu_{\text{Zr}} = \mu_{\text{ex}}^{\text{AlINiZr}} - X_{\text{Ni}} \frac{\partial \mu_{\text{ex}}^{\text{AlINiZr}}}{\partial X_{\text{Ni}}} - (1 - X_{\text{Zr}}) \frac{\partial \mu_{\text{ex}}^{\text{AlINiZr}}}{\partial X_{\text{Zr}}}$$  \hspace{1cm} (22)
3. Experiments and Results

Zirconium and aluminum layers (each 1 µm thick) were deposited by the EB-PVD method [18]. The samples with Zr and Al layers were subjected to diffusion treatment at 1325 K for 4 h in the argon atmosphere.

The microstructure of the coating was examined by the use of an optical microscope Nikon Epiphot 300, a scanning electron microscope (SEM) Hitachi S-3400N and an energy dispersive spectroscopy (EDS) Fig.2.

The coating consists two zones: outer (3-4 µm thick) zone and internal (6-7 µm thick) one. On the top of the coating the proportion of Ni, Al and Zr corresponded to Ni(Al,Zr) phase (Fig. 2, Table 1, Point 1). The chemical composition of the inner zone, distributed below the Ni(Al,Zr) phase corresponds to the Ni$_5$Zr phase (Fig. 2, Table 1 Point 2). Below the presence of the Ni(Al,Zr) phase was detected (Fig. 2, Table 1, Point 3).

![Figure 2. Microstructure of the Zr 1 µm thick and Al 1 µm thick coatings deposited by EB-PVD method after diffusion treatment.](image)

<table>
<thead>
<tr>
<th>Point</th>
<th>Chemical composition, % at</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Al</td>
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<tr>
<td>2</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>2.91</td>
</tr>
</tbody>
</table>

Table 1. Chemical composition on the cross-section of the Zr 1 µm thick and Al 1 µm thick coatings after diffusion treatment

When zirconium content is high the diffusion coefficients in γ-Ni phase based is on Campbell approximation[19]. The diffusion between γ-Ni and Ni$_5$Zr phase is analyzed. The
Zr diffusion coefficient is approximated basing on the Grandjean and Limoge data[20], Table 2.

Table 2. Thermodynamic and kinetic data used to simulate the reactions in Ni-Al-Zr system at 1325 K.

<table>
<thead>
<tr>
<th>Phase, j</th>
<th>Al diffusion coefficient, $D_{Al,j}$ [cm$^2$s$^{-1}$]</th>
<th>Ni diffusion coefficient, $D_{Ni,j}$ [cm$^2$s$^{-1}$]</th>
<th>Zr diffusion coefficient, $D_{Zr,j}$ [cm$^2$s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma$-Ni</td>
<td>4.24 $10^{-12}$</td>
<td>4.24 $10^{-12}$</td>
<td>10$^{-15}$</td>
</tr>
<tr>
<td>ZrNi$_5$</td>
<td>4.24 $10^{-12}$</td>
<td>4.24 $10^{-12}$</td>
<td>10$^{-15}$</td>
</tr>
</tbody>
</table>

Figures 3 and 4 present the time evolution of the concentration profile and the diffusion path. The presented data describe changes of the average composition of the system parallel to the mass transport direction, as it results from the concentration profiles. It is seen that the diffusion path passes the $\gamma = Ni + Ni_5Zr$ two-phase region. This means that such two-phase zone might grow during diffusion. The points where the diffusion path cross the interphase boundaries determine the average compositions of the system for which any phase (dis)appear or one phase transform into the other.

Figure 3. The comparison of the concentration profile of the NiAlZr multiphase diffusion experiments (dots) and simulations (line).
Figure 4. The comparison of the concentration profile of the NiAlZr multiphase diffusion experiments and simulations on a concentration triangle. Two phase can be distinguish: $\gamma$-Ni and Ni$_5$Zr phase.

5. Conclusion.

Based on the bi-velocity method, a model of reactive diffusion in three-component systems was proposed. The model is based on the generalized Darken approach with proper boundary conditions. The generalized Darken method is coupled with the phase field approach. The model includes both drift and diffusion velocities. The presented results are used to model the zirconium doped aluminate coatings formation deposited on pure nickel by the PVD method. It was shown that Zr behaves as a marker. Results of simulation well describe experimental values of nickel, aluminum and zirconium concentration distribution in zirconium dopped alumina coatings.

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Component Analysis in Financial Time Series

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Abstract: In this work we consider the application of some signal processing techniques to multivariate financial time series, particularly the Principal Component Analysis (PCA), the Independent Component Analysis (ICA), also known as blind source separation and the quite recent Forecastable Component Analysis (ForeCA). The key idea is not to compare their differences but more to find their “joint strenght” by joining their different views of time series. Knowing, for instance, that ICA linearly maps the observed multivariate time series into a new space of statistically independent components (ICs) we could “observe” the other two techniques at the same “time” and merge the information. We applied these techniques to two different scenarios: one, more micro, to some stocks quoted in the Portuguese Stock Market (PSI20); the other one, more macro, to study nine European stock markets.

Keywords: Data reduction, Stock Market, Pearson Correlation, Distance Covariance, Component Analysis

1. Introduction

In 1967, a seminal paper on the spectrum of empirical correlation matrices written by Marcenko and Pastur turned out to be useful in many and very different contexts like, for our purposes, finance time series. Its central objective, as a new statistical tool to analyze large dimensional data sets, only became fully relevant in the last twenty years, when the storage and handling of great amounts of data became a daily routine in financial markets.

The correlations within stock price fluctuations for different assets or markets are important because, for instance, of their direct use for risk management in the Markowitz portfolio theory. In this study, however, in a less profitability use, we are more interested in collecting the real information from stocks dependency. In practice, there are different sources of noise in the estimated correlations.

In their work, Laloux et. al., show that this accumulated noise in the correlation matrix for price fluctuations can be accounted for by using the tools from the random matrix theory (RMT). In particular, they found that the distribution of eigenvalues of empirical correlation matrix, excluding some of the largest

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eigenvalues, fits very well in the Marcenko-Pastur distribution of the RMT. These results strongly suggest that eigenvalues of correlation matrix falling under the Marcenko-Pastur distribution contain no genuine information about the financial markets. Extended work has been conducted to explain information contained in the deviating eigenvalues, which reveals that the largest eigenvalue corresponds to a market wide influence to all stocks and the remaining deviating eigenvalues correspond to conventionally identified business sectors. Using the same RMT method, extensive works have been performed in the correlation analysis of various stock markets.

In this work we are going to retrieve some of these results using RMT applied to two sets: first to twelve stocks quoted in the Portuguese Stock Market (PSI20) and then to nine European stock markets. Finally, we will apply Principal Component Analysis (PCA), Independent Component Analysis (ICA) and Foresectable Component Analysis (ForeCA) to these same sets in an effort to merge the resulting information.

2. Methods

2.1 Principal Component Analysis (PCA)

PCA is defined as a statistical procedure that by means of an orthogonal transformation converts a set of observations of (possibly correlated) variables into a set of linearly uncorrelated variables called principal components. This transformation is defined in such a way that the first principal component has the largest possible variance. The remaining components in turn have the highest variance possible under the constraint that it is orthogonal (uncorrelated with) to the preceding components. Principal components are guaranteed to be independent if the data set is jointly normally distributed.

PCA invention is attributed to Karl Pearson (1901) who created this as an analogue of the principal axes theorem in mechanics; it was later independently developed and named by Harold Hotelling in the 1930s. The method is mostly used as a tool in exploratory data analysis and for making predictive models.

PCA is considered the simplest of the true eigenvector-based multivariate analyses and here we will use the eigenvalue decomposition of the data covariance (or correlation) matrix, being in that way, closely related to the RMT method.

2.2 Independent Component Analysis (ICA)

The method known as independent component analysis (ICA) is also referred to as blind source separation (Herault and Jutten 1986, Jutten and Herault 1991, Comon 1994). The central assumption is that an observed multivariate time
series (daily stock returns) reflect the reaction of a system (the stock market) to a few statistically independent time series. ICA seeks to extract out these independent components as well as the mixing process. Here we will follow Back and Weigend (1997) approach to express ICA in terms of other measures of the statistical independence of signals.

In financial context, ICA was proposed for the first time by Moody and Wu to separate the observational noise from the true price in a foreign exchange rate time series.

![Figure 1: Schematic representation of ICA](image)

The original sources are mixed through matrix to form the observed signal. The demixing matrix transforms the observed signal into the independent components. Figure 1 shows the most basic form of ICA. We observe a multivariate time series, consisting of values at each time step. We assume that it is the result of a mixing process.

We will consider here the application of a signal processing technique known as independent component analysis (ICA) or blind source separation. This technique can be applied to multivariate financial time series and the main idea is to linearly map the observed multivariate time series into a new space of statistically independent components.

ICA versus PCA

Independent component analysis can be contrasted with principal component analysis and so we give here a brief comparison of the two methods here. Both ICA and PCA linearly transform the observed signals into components. The key difference however, is in the type of components obtained.

PCA algorithms use only second order statistical information. On the other hand, ICA algorithms may use higher order statistical information for separating the signals. For this reason non-Gaussian signals (or at most, one Gaussian signal) are normally required for ICA algorithms based on higher order statistics. For PCA algorithms however, the higher order statistical information provided by such non-Gaussian signals is not required or used, hence the signals in this case can be Gaussian.
2.3 Forecastable Component Analysis (ForeCA)

Here we introduce Forecastable Component Analysis (ForeCA), a novel dimension reduction technique for temporally dependent signals (Goerg, 2013). Based on a new forecastability measure, ForeCA finds an optimal transformation to separate a multivariate time series into a forecastable and an orthogonal white noise space. We will the R package ForeCA, which uses a converging algorithm with a fast eigenvector solution. Applications to financial and macro-economic time series show that ForeCA can successfully discover informative structure, which can be used for forecasting as well as classification.

3. Data and Results

3.1 The PSI-20 set

The 12 stocks that we call the PSI-20 set were obtained from the PSI-20 Index which is a price index calculation based on 20 stocks obtained from the universe of Portuguese companies listed to trade on the Main Market and was designed to became the underlying element of futures and options contracts. The data used in this study are the close values and its log returns from these 12 stocks, and cover the period from January 24, 2000 to September 25, 2013 for a total of 3362 observations. In Figure 2 we can see the daily values from the PSI-20 index.

Figure 2: PSI-20 from 2001 to 2014

During the period 1997-2001 the Portuguese stock market becomes highly sensitive to fluctuations in international markets due to the integration in the euro area markets. Moreover, the reduced size of the Portuguese financial market suggests that the behavior of national stock returns depends highly or mimics the behaviors of stock returns in European and American markets. The period from January 2001 and November 2001 was characterized by economical and political instability in Europe and United States due to the introduction of euro and the high value of the dollar against the euro, some regional conflicts like the Israel- Palestinian conflict, and the September 11 with negative impacts
on the financial markets, including the Portuguese stock market. In this period the PSI-20 index declined by 24.42 per cent. Between 2002 and 2007 we assisted to markets recovery, but in 2008, with the mortgage and subprime crises we saw the world markets in general, and PSI-20 in particular, going down once again. Finally, we are having some recovery signals from the beginning of 2013.

Calculating the Correlation Matrix using the Statistical Software R, we obtain for these 12 stocks:

<table>
<thead>
<tr>
<th>CorM</th>
<th>1.00</th>
<th>0.84</th>
<th>0.80</th>
<th>0.45</th>
<th>0.12</th>
<th>0.64</th>
<th>-0.00</th>
<th>0.02</th>
<th>0.39</th>
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<th>0.47</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.84</td>
<td>1.00</td>
<td>0.75</td>
<td>0.52</td>
<td>0.21</td>
<td>0.68</td>
<td>0.24</td>
<td>0.10</td>
<td>0.40</td>
<td>-0.06</td>
<td>0.49</td>
<td>0.33</td>
<td></td>
</tr>
<tr>
<td>0.80</td>
<td>0.75</td>
<td>1.00</td>
<td>0.61</td>
<td>0.04</td>
<td>0.49</td>
<td>-0.04</td>
<td>0.28</td>
<td>0.36</td>
<td>0.07</td>
<td>0.50</td>
<td>0.56</td>
<td></td>
</tr>
<tr>
<td>0.45</td>
<td>0.52</td>
<td>0.61</td>
<td>1.00</td>
<td>0.06</td>
<td>0.42</td>
<td>0.03</td>
<td>0.30</td>
<td>0.26</td>
<td>-0.00</td>
<td>0.45</td>
<td>0.18</td>
<td></td>
</tr>
<tr>
<td>0.12</td>
<td>0.21</td>
<td>0.04</td>
<td>0.06</td>
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<td>0.26</td>
<td>0.27</td>
<td>0.15</td>
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<tr>
<td>0.64</td>
<td>0.68</td>
<td>0.49</td>
<td>0.42</td>
<td>0.26</td>
<td>1.00</td>
<td>0.04</td>
<td>-0.04</td>
<td>0.48</td>
<td>0.15</td>
<td>0.35</td>
<td>0.09</td>
<td></td>
</tr>
<tr>
<td>-0.00</td>
<td>0.24</td>
<td>-0.04</td>
<td>0.03</td>
<td>0.27</td>
<td>0.04</td>
<td>1.00</td>
<td>0.09</td>
<td>0.19</td>
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<tr>
<td>0.02</td>
<td>0.10</td>
<td>0.28</td>
<td>0.30</td>
<td>0.15</td>
<td>-0.04</td>
<td>0.09</td>
<td>1.00</td>
<td>0.09</td>
<td>0.38</td>
<td>0.24</td>
<td>0.35</td>
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</tr>
<tr>
<td>0.39</td>
<td>0.40</td>
<td>0.36</td>
<td>0.26</td>
<td>0.28</td>
<td>0.48</td>
<td>0.19</td>
<td>0.09</td>
<td>1.00</td>
<td>0.21</td>
<td>0.25</td>
<td>0.21</td>
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<td>0.09</td>
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<td>0.38</td>
<td>0.21</td>
<td>1.00</td>
<td>0.18</td>
<td>0.29</td>
<td></td>
</tr>
<tr>
<td>0.54</td>
<td>0.49</td>
<td>0.50</td>
<td>0.45</td>
<td>0.52</td>
<td>0.35</td>
<td>-0.04</td>
<td>0.24</td>
<td>0.25</td>
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<td>1.00</td>
<td>0.60</td>
<td></td>
</tr>
<tr>
<td>0.47</td>
<td>0.33</td>
<td>0.36</td>
<td>0.18</td>
<td>0.50</td>
<td>0.05</td>
<td>-0.07</td>
<td>0.35</td>
<td>0.21</td>
<td>0.29</td>
<td>0.60</td>
<td>1.00</td>
<td></td>
</tr>
</tbody>
</table>

This matrix confirms some empirical ideas we had about the stocks, namely that the first and the second ones (“bes” and “bpi”) are highly correlated, which is not a surprise as these 2 stocks are from the financial sector. More surprisingly is the high correlation between each of these two and the third one (“edp”) that comes from electrical sector.

Calculating the relationship between the first three eigenvalues for 12 stocks: "bes", "bpi", "edp", "jeronimomartins", "motaengil", "novabase", "portucel", "portugalfutebolclub", "semapa", "sonaeC", "sonaeR" and "zonoptimus", and considering a sliding window of 20 days, we got the following:

From Figure 3 it is understandable that the ratio between the second eigenvalue (eigenvalue 2) and the first eigenvalue (eigenvalue 1), named eig12, has a global mean of 0.5, that is to say, the highest eigenvalue has a value that doubles the
second one. The mean for the eig13 is, for all the period, of about 0.39, that is to say that the first eigenvalue is two and a half times higher than the third one. Looking closer at the Figure3 we can observe that these ratios diminished greatly in the last six years: for eig12 the mean goes to 0.2 and for eig13 the mean goes to 0.15. These diminishing values tell us that the stocks are more correlated.

Comparing these results with twelve random stocks we get the following figure:

![Figure 4: eig12 vs random eig12 for PSI20 stocks](image)

Here, it is clear the difference between the eigenvalues from the random stocks (red) and the ones coming from the real stocks.

Performing Independent Component Analysis, following Back and Weigend (1997), for these stocks we can observe firstly their returns.

![Figure 5: returns for PSI20 stocks](image)

And then their independent components, obtained using the FastICA algorithm:
Finally, we work out a little bit of ForeCA. For our 12 stocks we obtain the following results:

We can see that all stocks have a Forecast value over 1.0%, and, from the two calculated components the most forecastable is ForeC2. For individual stocks we must refer the sixth, that is, “Novabase”.

3.2 European Markets set

The data used in this study was taken daily for a set of nine European market indices. We analyzed the following markets: Netherlands index (AEX), Austrian index (ATX), French index (CAC 40), German index (DAX 30), British index (FTSE 100), Spanish index (IBEX 35), Italian index (MIB), Portuguese index (PSI-20) and Swiss index (SSMI) from, roughly, the year 2000 until late September 2013.

The data used in this work are the daily Close values for these nine markets for a total of 3468 observations.
In Figure 8 we can observe the returns for the nine markets. It seems with no doubt that they are synchronized.
Looking at the returns helps us to look only to relative variation and not to absolute values. In fact, these markets are quite different in absolute values, as we can see from Figure 8.

![Figure 8: nine markets returns](image)

In order to perform a study using PCA we started by calculating and relatively compare their values for the 3 highest eigenvalues from the 9 markets. In Figure [fig:eig12vsEig13] we compare the relationship between the 3 major eigenvalues.

![Figure 9: eig12 (red) vs eig13 for the 9 markets](image)

We can generally say that the highest eigenvalue is getting higher over the time. It starts to be 3.3 to 5 times higher in the beginning of the XXI century and more recently became almost 10 to 15 times higher than the second. More recently, the difference between them is getting, again, smaller. From the second to the third highest we can infer a relationship of 2.
Performing Independent Component Analysis, following Back and Weigend (1997), for the nine markets we can observe their independent components, obtained using the FastICA algorithm:

Finally, we work out the results for markets of ForeCA. For our 9 markets we obtain the following results:

4. Conclusions

Indeed, PCA, ICA and ForeCA gives uses different but hopefully complementary views concerning the dependence and relationship between stocks or market indices.
Clearly, it is more difficult to get good insights when looking at stocks comparing with markets. These are much more correlated, something that we only see in stocks from the same sector.

Component analysis, despite being around for some time, deserves new approaches that a complementary view can offer. ForeCA gives us promising results and we hope to explore more in future work.

References


Step-wise Fractal Kinetics in Physical Ageing: 
Compositional Complexity in Network Glass-Formers

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Abstract. Sigmoid behavior of natural physical ageing in network glass-formers revealing multi-step-wise growing kinetics of enthalpy losses \(\Delta H(t)\) is studied at the example of glassy Se-rich arsenoselenides As-Se (As\(_{10}\)Se\(_{90}\), As\(_{20}\)Se\(_{80}\) and As\(_{30}\)Se\(_{70}\)). It is shown that phenomenological description of this ageing kinetics can be adequately developed in terms of first-order relaxation processes, tending atomic structure of a glass from initial towards more thermodynamically equilibrium state. The microstructure mechanism of natural physical ageing is explained by specificity of structural-topological complexes in the studied glasses (ratio between structural fragments having heteropolar As-Se and homopolar As-As and Se-Se covalent chemical bonds). This kinetics is shown to obey characteristic stretched exponential behavior originated from a number of growing steps, attributed to interconnected processes of chalcogen chains alignment and cooperative shrinkage of a whole glassy-like network. Developed model of natural physical ageing explains well the observed stretch-exponential behavior of low-temperature relaxation kinetics in terms of hierarchically-constrained mixed serial-parallel relaxation events having different atomic precursors, such as Se-based chains - Se-Se-Se-\(^=\), As-Se-Se-\(^=\) and =As-Se-As\(^=\). This phenomenological ageing kinetics can be decomposed into a few elementary components, each of them approaching to single exponential dependence.

Keywords: Chalcogenide Glasses, Physical Ageing, Differential Scanning Calorimetry, Glassy Network, Structural Fragments.
1. Introduction

The natural physical ageing (PhA) is known to be an important phenomenon for amorphous solids, because it results in uncontrolled time drift of such their important exploitation properties as atomic density, elastic modulus, brittleness, permeability, strength, fracture energy, deformation, etc. [1]. Nevertheless, the microstructural characteristics of PhA have not been studied enough, known only some reports related to PhA in silicate glasses [2-4]. However, the silicate glasses (characterized by over-constrained structural networks) possess very slow relaxation kinetics at ambient conditions [3] typically resulting in simple exponential dependence, which can be accepted only as a partial case for overall natural PhA kinetics.

From this point, the chalcogenide glasses (ChG) are more suitable objects for detailed examination of PhA kinetics, because they allow studying of almost complete picture of PhA at quite acceptable timescales ranging from a few days or even hours (in the case of very chalcogen-rich compositions) up to years or even decades (in case of chalcogen-depleted compositions) [5-7].

In general, the compositional variations in the ability to PhA are determined by a number of Lagrangian constraints per atom $n_c$ of ChG-forming networks built of fully-saturated covalent chemical bonds assuming their equivalence with movement stretching and bending limitations (mechanical constraints). Under this definition, the covalent bonding $Z$ can be described by mean number of covalent bonds per one atom of glass-forming network. The under-constrained networks possessing $Z < 2.4$ and smaller $n_c$, which are less than dimensionality of space $n_c < 3$, are subject to pronounced drift in their properties caused by thermodynamically-driven forces tending the system towards more favorable energetic state. In contrast, the over-constrained ($Z > 2.4$, $n_c > 3$) and optimally-constrained ($Z = 2.4$, $n_c = 3$) ChG do not age at normal conditions at all, demonstrating strong non-ageing ability.

In this paper, the kinetics peculiarities of natural PhA will be studied in under-constrained of As$_{10}$Se$_{90}$ ($Z = 2.1$, $n_c = 2.25$), As$_{20}$Se$_{80}$ ($Z = 2.2$, $n_c = 2.5$) and As$_{30}$Se$_{70}$ ($Z = 2.3$, $n_c = 2.75$) ChG and comparative analysis will be developed for this compositional row of glass formers taking into account their main structural features in respect to previously analyzed [6].

2. Experimental

The ChG of binary As$_x$Se$_{100-x}$ ($x = 10, 20, 30$) system were prepared by conventional melt-quenching route in the evacuated quartz ampoules from a mixture of high-purity elemental precursors, as described elsewhere [7]. Amorphous state and composition of the as-prepared ChG were controlled visually by a characteristic conch-like fracture, data of X-ray diffraction and X-ray photoelectron spectroscopy. Bulk samples in the form of thick (~3 mm) plates, prepared for differential scanning calorimetry (DSC) measurements, were used for the investigations.
DSC measurements were performed using NETZSCH 404/3/F microcalorimeter pre-calibrated with a set of standard elements, the DSC traces being recorded in ambient atmosphere with $q = 5 \text{ K/min}$ heating rate. More detailed description of the measurements protocol can be found in [7].

3. Results

The curve of time-dependent enthalpy losses $\Delta H(t)$ in As$_{10}$Se$_{90}$ ChG associated with long-term PhA is presented on Fig. 1.

As it follows from Fig. 1, the kinetic of PhA in As$_{10}$Se$_{90}$ ChG exhibits well-expressed four-steps character. The straightforward fitting of the experimental data describing enthalpy losses $\Delta H(t)$ in this As$_{10}$Se$_{90}$ glass during natural PhA with the stretched-exponential relaxation function gives numerical values of time constant $\tau \cong 663$ days and power index (index of non-exponentionality or dispersivity) $\beta = 0.25$. Taking into account that this kinetics is characterized by hierarchically-constrained mixed serial-parallel relaxation behavior, it can be conveniently modeled by the following expression:

$$
\Delta H_i(t) = \sum_{\beta=1}^{n} \theta(t - \Delta t_i) \left[ a_i + b_i (1 - \exp \left( -\frac{t - \Delta t_i}{\tau_i} \right) ) \right],
$$

(1)
where $a_i$ and $b_i$ are materials-related parameters connected with amplitude of the relaxation process, $\tau_i$ is effective time constant (the relaxation time), $\Delta t_i$ is a so-called retardation time (the parameter giving time delaying of the next step of PhA in respect to the previous one), $\Theta(t-\Delta t_i)$ is the Heaviside step function, whose value is accepted to be 0 for negative arguments ($t < \Delta t_i$) and 1 for positive arguments ($t \geq \Delta t_i$), and $n$ is number of steps in the relaxation kinetics.

The results of the modelling with eq. (1) and corresponding fitting parameters for four-steps serial presentation of PhA in As$_{10}$Se$_{90}$ ChG are given in Table 1.

Table 1. Fitting parameters in eq. (1), describing PhA kinetics in As$_{10}$Se$_{90}$ ChG.

<table>
<thead>
<tr>
<th>Step # (duration, days)</th>
<th>Fitting goodness $r^2$</th>
<th>$a_i$, J/g</th>
<th>$b_i$, J/g</th>
<th>$a_i+b_i$, J/g</th>
<th>$\tau_i$, days</th>
<th>$\Delta t_i$, days</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i=1$ (0+1.5)</td>
<td>0.008</td>
<td>0</td>
<td>0.46</td>
<td>0.46</td>
<td>0.2</td>
<td>0</td>
</tr>
<tr>
<td>$i=2$ (1.5+20)</td>
<td>0.022</td>
<td>0.46</td>
<td>1.52</td>
<td>1.98</td>
<td>5.3</td>
<td>1.7</td>
</tr>
<tr>
<td>$i=3$ (20+365)</td>
<td>0.038</td>
<td>1.98</td>
<td>1.82</td>
<td>3.80</td>
<td>35.0</td>
<td>16.5</td>
</tr>
<tr>
<td>$i=4$ (365+10000)</td>
<td>0.034</td>
<td>3.80</td>
<td>3.27</td>
<td>7.07</td>
<td>1173</td>
<td>340</td>
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</table>

The curve of time-dependent enthalpy losses $\Delta H(t)$ in As$_{20}$Se$_{80}$ ChG associated with long-term PhA is presented below on Fig. 2.

![Fig. 2. Kinetics of $\Delta H(t)$ losses in As$_{20}$Se$_{80}$ ChG decomposed in three-steps serial single-exponential processes](image-url)
The kinetic of PhA in As$_{20}$Se$_{80}$ ChG exhibits two-steps behaviour, the values of PhA is expected smallest as compared with the same in As$_{10}$Se$_{90}$ ones (number of constrains per atom $n_c = 2.5$). The straightforward fitting of the experimental data describing enthalpy losses $\Delta H(t)$ in As$_{30}$Se$_{70}$ ChG during PhA with stretched-exponential relaxation function gives $\tau = 1008.6$ days and $\beta = 0.28$. The results of the modelling with eq. (1) and fitting parameters for this three-step serial presentation of PhA kinetics in As$_{20}$Se$_{80}$ ChG are gathered in Table 2.

Table 2. Fitting parameters in eq. (1) describing PhA kinetics in As$_{20}$Se$_{80}$ ChG.

<table>
<thead>
<tr>
<th>Step # (duration, days)</th>
<th>Fitting goodness $r^2$</th>
<th>$a_i$, J/g</th>
<th>$b_i$, J/g</th>
<th>$a_i+b_i$, J/g</th>
<th>$\tau$, days</th>
<th>$\Delta \tau$, days</th>
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<tr>
<td>$i=1$ (1÷20)</td>
<td>0.0933</td>
<td>0</td>
<td>1.4</td>
<td>1.4</td>
<td>4.9</td>
<td>0</td>
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<tr>
<td>$i=2$ (20÷335)</td>
<td>0.03705</td>
<td>1.4</td>
<td>2.0</td>
<td>3.4</td>
<td>66.8</td>
<td>17.5</td>
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<tr>
<td>$i=3$ (335÷10000)</td>
<td>0.04821</td>
<td>3.4</td>
<td>2.7</td>
<td>6.1</td>
<td>1651.4</td>
<td>305</td>
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</table>

The curve of time-dependent enthalpy losses $\Delta H(t)$ in As$_{30}$Se$_{70}$ ChG associated with long-term PhA is presented on Fig. 3.
The kinetic of PhA in As$_{30}$Se$_{70}$ ChG exhibits two-steps behaviour, the values of PhA is expected smallest as compared with the same in As$_{10}$Se$_{90}$ and As$_{20}$Se$_{80}$ ones (the number of constrains per one atom $n_c = 2.75$). The straightforward fitting of the experimental data describing enthalpy losses $\Delta H(t)$ in As$_{30}$Se$_{70}$ ChG during PhA with the stretched-exponential relaxation function gives $\tau \approx 100242.7$ days and $\beta = 0.35$. The results of modelling with eq. (1) and fitting parameters for two-steps serial presentation of PhA kinetics in As$_{30}$Se$_{70}$ ChG are gathered below in Table 3.

Table 3. Fitting parameters in eq. (1) describing PhA kinetics in As$_{30}$Se$_{70}$ ChG.

<table>
<thead>
<tr>
<th>Step # (duration, days)</th>
<th>Fitting goodness $r^2$</th>
<th>$a_i$, J/g</th>
<th>$b_i$, J/g</th>
<th>$a_i + b_i$, J/g</th>
<th>$\tau$, days</th>
<th>$\Delta t$, days</th>
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<tr>
<td>i=1 (1+300)</td>
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<td>0.7</td>
<td>0.7</td>
<td>-</td>
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<tr>
<td>i=2 (300+10000)</td>
<td>0.0265</td>
<td>0.7</td>
<td>3.3</td>
<td>4</td>
<td>1398</td>
<td>250</td>
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</table>

4. Discussion

The mechanism of PhA in ChG is known to be based on elementary relaxation acts (twisting) of inner Se atoms within double-well potentials associated with high flexibility of chalcogen chemical bonds [7-9].

As it follows from above experimental results, the PhA in the studied ChG exhibits well-expressed step-wise character, showing some kinds of plateaus and steep regions. The increasing of As content leads to decreasing of PhA in full accordance to increased $n_c$ values (from 2.25 for As$_{10}$Se$_{90}$ to 2.5 for As$_{20}$Se$_{80}$ and 2.75 for As$_{30}$Se$_{70}$ ChG). Moreover, with increase in As content, the values of non-exponentionality index $\beta$ in the stretched-exponential relaxation function describing observed kinetics increases (from 0.25 for As$_{10}$Se$_{90}$ to 0.28 for As$_{20}$Se$_{80}$ and 0.36 for As$_{30}$Se$_{70}$ ChG). This means, obviously, the decrease in the dispersivity of the system, so the number of steps in the PhA kinetics decreases too (from 4 for As$_{10}$Se$_{90}$ to 3 for As$_{20}$Se$_{80}$ and 2 in As$_{30}$Se$_{70}$ ChG).

These features can be well explained by accepting main microstructure signatures of the studied ChG.

Thus, in As$_{10}$Se$_{90}$ ChG, the Se atoms created -Se-Se-Se- chains ($n_c = 2.0$) and $\equiv$As-Se-Se- ($n_c = 2.45$) fragments taken in 67:33 ratio, while in As$_{20}$Se this ratio become only 25:75. In contrast, in As$_{30}$Se$_{70}$ ChG, the intermediate surroundings of Se atoms significantly changes: -Se-Se-Se- chains disappear, and principally new $\equiv$As-Se-$\equiv$ ($n_c = 3.00$) structural environment is formed instead (the ratio between $\equiv$As-Se-Se- and $\equiv$As-Se-$\equiv$ structural fragments reaches as high as 29:71).

Under such conditions, three types of double-well potentials can be assumed for central Se atoms in the studied ChG owing to their immediate surroundings,
namely -Se-Se-Se-, =As-Se-Se- and =As-Se-As= fragments with differing heights of energetic barriers.

It is well known that -Se-Se-Se- fragments possess the smallest height of energetic barrier, while =As-Se-As= fragments are characterized by the highest barrier. Therefore, -Se-Se-Se- fragments relax on the initial stages of PhA with characteristic time constant $\tau \sim 4.9$ days, and =As-Se-As= fragments relax at the final stage of natural PhA with characteristic time constant $\tau \sim 1200 \div 1600$ days (see Tables 1-3), although (according to serial-parallel specificity of long-term natural PhA) the relaxation of all structural fragments present in the glass occurs on each stage.

Since the content of -Se-Se-Se- structural fragments in $\text{As}_{20}\text{Se}_{80}$ ChG (25 %) is less that in $\text{As}_{10}\text{Se}_{90}$ (67 %) [7], the initial two steps in $\text{As}_{20}\text{Se}_{80}$ glasses arise very quickly. Therefore, its separate distinction is not possible under such condition (see Fig. 2), and, consequently, both first and second steps cooperate giving the smallest value of time constant $\tau$.

In case of $\text{As}_{30}\text{Se}_{70}$ ChG, the homoatomic -Se-Se-Se- structural fragments are absent at all, and initial stage of relaxation are caused mainly by shrinkage of =As-Se-Se- structural fragments, producing only two steps in the final relaxation kinetics.

It should be noted that the retardation times $\Delta t_i$ in eq. (1) remain on the same order for all types of relaxing atomic environments whichever the glass composition (Table 1-3).

**Conclusions**

It is shown that kinetics of enthalpy losses $\Delta H(t)$ caused by natural physical ageing in Se-rich As-Se ChG during more than two decades exhibited well-expressed step-wise behavior. The microstructure mechanism of this relaxation in the studied ChG is shown to be governed by structural-topological nature of corresponding glassy network.

**References**


Chaos in Pendulum Systems with Limited Excitation in the Presence of Delay

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Abstract. Dynamic system "pendulum - source of limited excitation" with taking into account the various factors of delay is considered. Different approaches to write a mathematical model of this system using three- or fifteen-dimensional systems of differential equations without delay is suggested. It is established that for small values of the delay it is sufficient to use three-dimensional mathematical model, whereas for relatively large values of the delay the fifteen-dimensional mathematical model should be used.

Genesis of deterministic chaos is studied in detail. Maps of dynamic regimes, phase portraits of attractors of systems, phase-parametric characteristics, Poincare sections and maps are constructed and analyzed. The scenarios of transition from steady-state regular regimes to chaotic ones are identified. It is shown, that in some cases the delay is the main reason of origination of chaos in the system "pendulum - source of limited excitation".

Keywords: pendulum system, limited excitation, delay, deterministic chaos.

1 Introduction

In mathematical modeling of oscillatory processes a mathematical model of a relatively simple dynamical system is often used to study the dynamics of much more complex systems. A typical example of this approach is the extensive use of pendulum models to study the dynamics of systems of an entirely different nature. Pendulum mathematical models are widely used to describe the dynamics of various technical constructions, machines and mechanisms, in the study of cardiovascular system, financial markets, etc. Such widespread use of pendulum models makes it relevant to study directly the dynamics of pendulum systems.

The study of the non-ideal by Zommerfeld–Kononenko [1] dynamical system "pendulum–electric motor" in the absence of any delay factors was initiated in [2], [3]. In this system the existence of deterministic chaos was identified and studied. It was proved that limited excitation is the main cause of chaos in this system.

In this paper the oscillations of “pendulum–electric motor” system with taking into account various factors of delay are considered. The delay factors are always present in rather extended systems due to the limitations of signal transmission speed: waves of compression, stretching, bending, current strength, etc. The aim of this work is to study the influence of various factors of delay on steady-state regimes of this system.
2 Delay factors in “Pendulum–electric motor” system

In the absence of any delay factors the equations of motion of the system “pendulum–electric motor” were obtained in [2]:

\[
\begin{align*}
\frac{dy_1}{d\tau} &= Cy_1 - y_2y_3 - \frac{1}{8}(y_1^2y_2 + y_2^3); \\
\frac{dy_2}{d\tau} &= Cy_2 + y_1y_3 + \frac{1}{8}(y_1^3 + y_1y_2^2); \\
\frac{dy_3}{d\tau} &= Dy_2 + Ey_3 + F;
\end{align*}
\]

where phase variables \(y_1, y_2\) describe the pendulum deviation from the vertical and phase variable \(y_3\) is proportional to the rotation speed of the motor shaft. The system parameters are defined by

\[
C = -\delta_1\varepsilon^{-2/3}\omega_0^{-1}, D = -\frac{2ml^2}{I}, F = 2\varepsilon^{-2/3}\left(\frac{N_0}{\omega_0} + E\right)
\]

where \(m\) - the pendulum mass, \(l\) - the reduced pendulum length, \(\omega_0\) - natural frequency of the pendulum, \(a\) - the length of the electric motor crank, \(\varepsilon = \frac{a}{I}\), \(\delta_1\) - damping coefficient of the medium resistance force, \(I\) - the electric motor moment of inertia, \(E, N_0\) - constants of the electric motor static characteristics.

Let us consider the following system of equations [4]:

\[
\begin{align*}
\frac{dy_1(\tau)}{d\tau} &= Cy_1(\tau - \delta) - y_2(\tau)y_1(\tau - \gamma) - \frac{1}{8}(y_1^2(\tau)y_2(\tau) + y_2^3(\tau)); \\
\frac{dy_2(\tau)}{d\tau} &= Cy_2(\tau - \delta) + y_1(\tau)y_3(\tau - \gamma) + \frac{1}{8}(y_1^3(\tau) + y_1(\tau)y_2^2(\tau)); \\
\frac{dy_3(\tau)}{d\tau} &= Dy_2(\tau - \gamma) + Ey_3(\tau) + F.
\end{align*}
\]

Positive constant parameter \(\gamma\) was introduced to account the delay effects of electric motor impulse on the pendulum. We assume that the delay of the electric motor response to the impact of the pendulum inertia force is also equal to \(\gamma\). Taking into account the delay \(\gamma\) conditioned by the fact that the wave velocity perturbations on the elements of the construction has a finite value that depends on the properties of external fields, for instance, the temperature field. In turn, the constant positive parameter \(\delta\) characterizes the delay of the medium reaction on the dynamical state of the pendulum. This delay is due to the limited sound velocity in that medium.

Assuming a small delay, we can write

\[
\begin{align*}
y_i(\tau - \gamma) &= y_i(\tau) - \frac{y_i(\tau)}{d\tau}\gamma + \ldots, \quad i = 2, 3 \\
y_i(\tau - \delta) &= y_i(\tau) - \frac{y_i(\tau)}{d\tau}\delta + \ldots, \quad i = 1, 2
\end{align*}
\]
Then, if $C\delta \neq -1$, we get the following system of equations [4]:

$$
\begin{align*}
  y_1 &= \frac{1}{1+C\delta} \left( C y_1 - y_2 [y_3 - \gamma (Dy_2 + Ey_3 + F)] - \frac{1}{8}(y_1^2 y_2 + y_2^3) \right); \\
  y_2 &= \frac{1}{1+C\delta} \left( C y_2 + y_1 y_3 - y_1 \gamma (Dy_2 + Ey_3 + F) + \frac{1}{8}(y_1^3 + y_1 y_2^2) + 1 \right); \\
  y_3 &= (1-C\gamma)Dy_2 - \frac{D\gamma}{8}(y_1^3 + y_1 y_2^2 + 8y_1 y_3 + 8) + Ey_3 + F.
\end{align*}
$$

(4)

The obtained system of equations is already a system of ordinary differential equations. Delays are included in this system as additional parameters.

In order to approximate the system (3) another, more precise, method can be used [5], [6]. Let us divide each of the segments $[\gamma; 0]$ and $[-\delta; 0]$ into $m$ equal parts. We introduce the following notation

$$
\begin{align*}
  y_1(\tau - \frac{i\delta}{m}) &= y_{i1}(\tau), \ y_2(\tau - \frac{i\gamma}{m}) = y_{i2}(\tau), \ y_2(\tau - \frac{i\delta}{m}) = \tilde{y}_{i2}(\tau), \\
  y_3(\tau - \frac{i\gamma}{m}) &= y_{i3}(\tau), \ i = 0, m.
\end{align*}
$$

Then, using difference approximation of derivative [5], [6] the system of equations with delay (3) can be reduced to the following system of equations without delay:

$$
\begin{align*}
  \frac{dy_{10}(\tau)}{d\tau} &= C y_{1m}(\tau) - y_{20}(\tau)y_{3m}(\tau) - \frac{1}{8}(y_{10}^2 y_{20}(\tau) + y_{20}^3(\tau)); \\
  \frac{dy_{20}(\tau)}{d\tau} &= C \tilde{y}_{2m}(\tau) + y_{10}(\tau)y_{3m}(\tau) + \frac{1}{8}(y_{10}^3(\tau) + y_{10}(\tau)y_{20}^2(\tau)) + 1; \\
  \frac{dy_{30}(\tau)}{d\tau} &= D y_{2m}(\tau) + Ey_{3m}(\tau) + F; \\
  \frac{dy_{i1}(\tau)}{d\tau} &= \frac{m}{\delta} (y_{i-1} - y_{i1}(\tau)), \ i = 1, m; \\
  \frac{dy_{i2}(\tau)}{d\tau} &= \frac{m}{\gamma} (y_{i-1} - y_{i2}(\tau)), \ i = 1, m; \\
  \frac{d\tilde{y}_{i2}(\tau)}{d\tau} &= \frac{m}{\delta} (\tilde{y}_{i-1} - \tilde{y}_{i2}(\tau)), \ i = 1, m; \\
  \frac{dy_{i3}(\tau)}{d\tau} &= \frac{m}{\gamma} (y_{i-1} - y_{i3}(\tau)), \ i = 1, m.
\end{align*}
$$

(5)

Should be noted that the main variables in this system are only $y_{10}$, $y_{20}$, $y_{30}$. In other words the solutions $y_1, y_2, y_3$ of the system (3) are described by the functions $y_{10}, y_{20}, y_{30}$ of the system (5).

The system (5) is a system of ordinary differential equations of $(4m + 3)$-th order. Choosing a sufficiently large $m$ in the system (5), the system (3) will
be very well approximated by the system (5) [5]. In this paper the system of equation (5) was considered at $m = 3$. In this case, the system (5) has 15 equations. The calculations of cases $m > 3$, with a significant increase the number of equations, were also carried out. It was established, that increasing the number of equations has practically no effect on identification and description of steady-state regimes of “pendulum–electric motor” system. But it significantly increases the complexity of constructing characteristics, which are necessary for study the steady-state regimes of oscillations. Therefore, the use of mathematical model (5) at $m = 3$ is the most optimal for studying the influence of delay on regular and chaotic dynamics of “pendulum–electric motor” system.

3 Maps of dynamic regimes

Therefore, we obtained three-dimensional (4) and fifteen-dimensional (5) models each describing the system of equations with delay (3). These models are the systems of non-linear differential equations, so in general the study of steady-state regimes can be carried out only by using numerical methods and algorithms. The methodology of such studies is described in detail in [2].

In the study of dynamical systems the information about the type of steady-state regime of the the system depending on its parameters is crucial. This information can provide a map of dynamic regimes. It is a diagram on the plane, where two parameters are plotted on axes and the boundaries of different dynamic regimes areas are shown. The construction of dynamic regimes maps is based on analysis and processing of spectrum of Lyapunov characteristic exponents [2,7]. Where necessary, for more accurate determination of steady-state regime of the system, we study other characteristics of attractors: phase portraits, Poincare sections and maps, Fourier spectrums and distributions of the invariant measure.

Let us consider the behavior of the systems (4) and (5) when the parameters are $C = -0.1$, $D = -0.6$, $E = -0.44$, $F = 0.3$. In fig. 1 the maps of dynamic

![Maps of dynamic regimes](image)

**Fig. 1.** Maps of dynamic regimes
regimes are shown. The map in fig. 1a was built for three-dimensional model (4) and the map in fig. 1b was built for fifteen-dimensional model (5). These figures illustrate the effect of delays $\gamma$ and $\delta$ on changing the type of steady-state regime of the systems. The dark-grey areas of the maps correspond to equilibrium positions of the system. The light-grey areas of the maps correspond to limit cycles of the system. And finally, the black areas of the maps correspond to chaotic attractors.

We can notice a certain similarity the maps in fig.1a, b. In delay absence in these systems, the steady-state regime is stable equilibrium position. With an increase of the delay of the medium $\delta$ the type of steady-state regime of the systems (4) and (5) does not change. It still remains an equilibrium position (dark-grey areas in the figures). However, with an increase of the delay of interaction between pendulum and electric motor $\gamma$, the equilibrium position is replaced by the area of limit cycles with "mounted" area of chaos. With further increase of the delay $\gamma$, the attractor of both systems is again equilibrium position.
Let us study the dynamics of the system (4) and (5) at other values of the parameters. At $C = -0.1$, $D = -0.58$, $E = -0.6$, $F = 0.19$ the steady–state regime of both systems is limit cycle. In fig. 2a the map of dynamic regimes of three-dimensional system (4) and in fig. 2b the map of dynamic regimes of fifteen-dimensional system (5) are shown. At small values of the delays the steady-state regime of both systems does not change, it is periodic. The attractors are limit cycles (light-grey areas in the figures). With a further increase of the delay values the maps in fig. 2a, b are certainly different. At small values of the delay $\gamma$ and with increase of the delay $\delta$ the type of steady–state regime of the system (5) is replaced by chaotic regimes, whereas the type of steady–state regime of the system (4) does not change, it remains periodic. Further in both figures there are a rather wide area of chaos in which fairly narrow strips of periodic regimes are built in.

In fig. 2c, d the maps of dynamic regimes of respectively the system (4) and the system (5) at $C = -0.1$, $D = -0.53$, $E = -0.6$, $F = 0.19$ are constructed. In delay absence and at small values of the delays both systems have chaotic attractors (black areas in the figures). With an increase of the delay values the region of chaos is replaced by the region of periodic regimes. Then again chaos arises in the system. Further this area is replaced by the area of limit cycles.

As seen from the constructed maps of dynamic regimes, the dynamics of the system (4) and (5) is the same only for small values of the delay $\gamma$ and $\delta$. With an increase of the delays the differences of the dynamics of these systems is very significant.

4 Regular and chaotic dynamics

Let us study the types of regular and chaotic attractors that exist in the systems (4) and (5). We implement a horizontal section of the maps of dynamic regimes in fig.2c, d along the delay $\gamma$ at $\delta = 0.15$. In other words, let us consider the

Fig. 3. The dependence of maximal non-zero Lyapunov’s characteristic exponent (a), phase-parametric characteristic (b) of three-dimensional system (4)
behavior of the systems (4) and (5) when parameters are $C = -0.1$, $D = -0.53$, $E = -0.6$, $F = 0.19$ and the delays $\delta = 0.15$ and $0 \leq \gamma \leq 0.3$.

In fig. 3a,b the dependence of maximum non-zero Lyapunov’s characteristic exponent and phase-parametric characteristic of three-dimensional system (4) are shown respectively. These figures illustrate the influence of the delay of interaction between pendulum and electric motor $\gamma$ on chaotization of the system (4).

Let us construct the same characteristics at the same values of the parameters for fifteen-dimensional system (5). In fig. 4a,b respectively the dependence of maximum non-zero Lyapunov’s characteristic exponent and phase-parametric characteristic are shown.

![Fig. 4. The dependence of maximal non-zero Lyapunov’s characteristic exponent (a), phase-parametric characteristic (b) of fifteen-dimensional system (5)](image)

In fig.3a, 4a we can clearly see the presence of intervals $\gamma$ in which maximum Lyapunov exponent of the systems is positive. In these intervals the systems have chaotic attractors. The area of existence of chaos is clearly seen in phase-parametric characteristics of the systems. The areas of chaos in the bifurcation trees are densely filled with points. A careful examination of the obtained images allows not only to identify the origin of chaos in the systems, but also to describe the scenario of transition to chaos. So with a decrease of $\gamma$ there are the transitions to chaos by Feigenbaum scenario (infinite cascade of period-doubling bifurcations of a limit cycle). Bifurcation points for the delay $\gamma$ are clearly visible in each figures. These points are the points of approaches of the Lyapunov’s exponent graph to the zero line (fig.3a, 4a) and the points of splitting the branches of the bifurcation tree (fig.3b, 4b). In turn, the transition to chaos with an increase of the delay happens under the scenario of Pomeau-Manneville, in a single bifurcation, through intermittency.

A careful analysis of these figures allows to see qualitative similarity of the respective characteristics of the systems (4) and (5). However, with increasing the delay the differences in the dynamics of these systems become very signif-
icant. So for instance at $\gamma = 0.05$ the steady–state regime of the system (4) is limit cycle. While at this value of the delay the attractor of the system (5) is chaotic attractor. Conversely, for example at $\gamma = 0.11$ the system (4) has steady–state chaotic regime. While at this value of the delay the system (5) has periodic regime of oscillations.

This suggests that three-dimensional system of equations (4) should be used to study the system (3) only at very small values of the delay. With increasing values of the delay to study regular and chaotic oscillations of “pendulum–electric motor” system, fifteen-dimensional system of equations (5) should be used.

5 Conclusion

Various factors of delay have significant influence on the dynamics of “pendulum–electric motor” system. The presence of delay in such systems can affect the type of steady-state regime change. It is shown that for small values of the delay it is sufficient to use three-dimensional mathematical model, whereas for relatively high values of the delay the fifteen-dimensional mathematical model should be used.

In future research is planned to construct and research mathematical models of “pendulum–electric motor” system in the presence of variable in time delay factors.

References

Parameter Matching Using Adaptive Synchronization of Two Chua’s Oscillators: MATLAB and SPICE Simulations

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Abstract. In this paper, we use an adaptive synchronization technique for parameter matching with chaotic persistent excitation (PE). Two Chua’s oscillators, identical in every parameter except for one, are set up in a master/slave configuration where the slave’s mismatched parameter is adaptable. Using a Lyapunov function and incorporating the presence of PE, an adaptive control law is given to ensure exact parameter matching. A high-fidelity SPICE simulation model is given that incorporates commercially-provided macro models of the integrated circuits used and obviates the need for any user-defined functions. A voltage controlled inductor-gyrator is used as a tunable parameter made up of current feedback op amps (CFOAs). The performance of the adaptive controller is compared over a wide range of parameter values by using MATLAB simulations. SPICE and MATLAB simulations are run with realistic component tolerances to mimic a physical experiment.

Keywords: Chua’s oscillator, adaptive synchronization, parameter matching, inductor-gyrator, CFOA, chaotic simulation, SPICE, MATLAB, TINA-TI.

1 Introduction

Chua’s circuit has been extensively used to study various topics relating to chaos theory, including synchronization of coupled chaotic systems [13]. When two chaotic systems are not identical, synchronization becomes less trivial and various adaptive schemes are considered. For example, adaptive synchronization of Chua’s oscillator has been considered with adaptive observer design [5], parameter identification [19], and adaptive backstepping [6]. Many of the prior works are theoretical in nature, difficult to realize experimentally, and may not yield exact parameter matching [3]. To render adaptive synchronization of chaotic circuits closer to physical realization, Ref. [18] has provided SPICE simulations with ideal user defined functions for the adaptive controller. Ref. [8] has suggested circuit schematics to realize an adaptive controller for synchronization of uncertain and delayed chaotic systems, but it does not account for the non-ideal characteristics of integrated circuits such as the AD633.

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Adaptive synchronization of Chua’s oscillators can be categorized in two parts: adapting the control coupling between the two circuits or adapting one or more parameters of the Chua’s oscillators [4]. Both adaptive synchronization approaches have been digitally implemented for secure communication applications. The first approach is used to account for changes in signal strength [20], while the second approach introduces deliberate changes in the parameters as a way to send binary messages as a ‘key’ [4].

In this paper, we use an adaptive synchronization technique for parameter matching with chaotic PE. Two Chua’s oscillators, identical in every parameter except for one, are set up in a master/slave configuration where the slave’s mismatched parameter is adaptable. Using a Lyapunov function and incorporating the presence of PE, an adaptive control law is given to ensure exact parameter matching. Following Ref. [15], this paper uses analog circuit schematics, which exploit CFOAs, to implement the derived adaptive controller. Moreover, a high-fidelity SPICE simulation model is provided that incorporates commercially available macro models of various integrated circuits used and obviates the need for any user-defined functions. The performance of the adaptive controller is compared over a wide range of parameter values by using MATLAB simulations. SPICE and MATLAB simulations are run with realistic component tolerances to mimic a physical experiment. For experimental results that parallel the simulation studies of this paper, see Ref. [15].

2 System Model

2.1 Chua’s Oscillator

In this paper, an adaptive controller is designed to tune a parameter of the Chua’s oscillator shown in Figure 1. Various parameters of a Chua’s oscillator include $L$ as a linear inductor, $R$ and $R_0$ as linear resistors, $C_1$ and $C_2$ as linear capacitors, and others that correspond to the Chua’s diode. The state equations of the Chua’s oscillator are given by

$$\begin{align*}
\frac{dv_1}{dt} &= \frac{1}{C_1} \left( G (v_2 - v_1) - g(v_1) \right), \\
\frac{dv_2}{dt} &= \frac{1}{C_2} \left( G (v_1 - v_2) + i_L \right), \\
\frac{di_L}{dt} &= \frac{1}{L} \left( -v_2 - R_0 i_L \right),
\end{align*}$$

where $v_1$, $v_2$, and $i_L$ are voltage across $C_1$, voltage across $C_2$, and current through $L$, respectively, and $G$ is the conductance of the resistor $R$ ($G \equiv \frac{1}{R}$). Furthermore $g(\cdot)$ is the nonlinear voltage-current ($v$–$i$) characteristic of the Chua’s diode described by

$$g(v_R) = \begin{cases} 
G_b v_R + (G_b - G_a) E_1, & \text{if } v_R \leq -E_1, \\
G_a v_R, & \text{if } |v_R| < E_1, \\
G_b v_R + (G_a - G_b) E_1, & \text{if } v_R \geq E_1,
\end{cases}$$

where $G_a$, $G_b$, and $E_1$ are known real constants that satisfy $G_b < G_a < 0$ and $E_1 > 0$. 

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2.2 Master/slave System

The adaptive control framework of this paper considers a unidirectional coupling from a master Chua’s oscillator to a slave Chua’s oscillator such that the slave Chua’s oscillator synchronizes its states to the states of the master oscillator which operates autonomously. This configuration is shown in Figure 1 where it is assumed that the following parameters of the master and slave Chua’s oscillators are matched, \( \tilde{R} = R, \tilde{R}_0 = R_0, \tilde{C}_1 = C_1, \) and \( \tilde{C}_2 = C_2. \) The state equations of the master Chua’s oscillator are equivalent to (1) while the state equations of the slave Chua’s oscillator are given by

\[
\begin{align*}
\frac{d\tilde{v}_1}{dt} &= \frac{1}{C_1} \left( G(\tilde{v}_2 - \tilde{v}_1) - g(\tilde{v}_1) + G_{u_1}(v_{u_1} - \tilde{v}_1) \right), \\
\frac{d\tilde{v}_2}{dt} &= \frac{1}{C_2} \left( G(\tilde{v}_1 - \tilde{v}_2) + \tilde{i}_L \right), \\
\frac{d\tilde{i}_L}{dt} &= \frac{1}{\tilde{L}} (-\tilde{v}_2 - R_0 \tilde{i}_L),
\end{align*}
\]

where \( v_{u_1} = v_1 \) since it is the output of a voltage follower op-amp and \( G_{u_1} \) is the conductance of the coupling resistor \( R_{u_1} \) in Figure 1 \( (G_{u_1} \triangleq \frac{1}{R_{u_1}}) \). Note that \( \tilde{L} \) is a tunable parameter for which we give an adaptive parameter update law in Section 3.

3 Adaptive Synchronization: Tuning \( \tilde{L} \)

In a master/slave configuration, the master Chua’s oscillator is described by (1). For the slave Chua’s oscillator, inductance \( \tilde{L} \) is the tunable mismatched parameter for the slave Chua’s oscillator (3). Subtracting (1) from (3) produces the error dynamics

\[
\begin{align*}
\dot{e}_{v_1} &= \frac{1}{C_1} \left( G(e_{v_2} - e_{v_1}) - c(\tilde{v}_1, v_1) e_{v_1} + u_1 \right), \\
\dot{e}_{v_2} &= \frac{1}{C_2} \left( G(e_{v_1} - e_{v_2}) + e_{i_L} \right), \\
\dot{e}_{i_L} &= \frac{1}{L} (-\tilde{v}_2 - R_0 i_L) + \frac{1}{L} (v_2 + R_0 i_L),
\end{align*}
\]

Fig. 1. Master/slave Chua’s oscillator coupling.
where \( e_{v_1} \triangleq \tilde{v}_1 - v_1 \), \( e_{v_2} \triangleq \tilde{v}_2 - v_2 \), and \( e_{i_L} \triangleq \tilde{i}_L - i_L \) are the error states and \( u_1 \triangleq G_{u_1}(v_1 - \tilde{v}_1) \). Moreover, it is easy to show that \( g(\tilde{v}_1) - g(v_1) = c(\tilde{v}_1, v_1)e_{v_1} \) where \( c(\tilde{v}_1, v_1) \) is bounded by the constraints \( G_a \leq c(\tilde{v}_1, v_1) \leq G_b < 0 \,[7] \).

Next, let the control law and parameter update law, respectively, be given by

\[
\mathcal{S} = -G_{u_1} e_{v_1} \quad \text{and} \quad \frac{d}{dt} \left( \frac{1}{\tilde{L}} \right) = \gamma e_{i_L} \left( \tilde{v}_2 + R_0 \tilde{i}_L \right),
\]  

(5)

where \( \gamma \) is a positive constant.

**Theorem 1.** [15] The two Chua’s oscillators (1) and (3) will synchronize and the parameter \( \tilde{L} \) will converge to some constant under (5) if the master system (1) remains on the trajectory of its chaotic attractor and \( G_{u_1} \) is chosen to satisfy the following inequality

\[
G_{u_1} > \frac{1}{2} G - G_a.
\]  

(6)

**Remark 1.** Note that the results of Theorem 1 are also applicable if the Chua’s oscillator is on a periodic trajectory. As long as the attractor of the Chua’s oscillator is bounded, the results of Theorem 1 hold.

**Remark 2.** When the trajectories of (1) are driven on a chaotic attractor, its states will satisfy the qualities of PE as discussed in [10,11,14] and \( \tilde{L}(t) \rightarrow L(t) \) as \( t \rightarrow \infty \). Further evidence of \( \tilde{L}(t) \rightarrow L(t) \) as \( t \rightarrow \infty \) is provided via simulation results in the sequel.

### 4 Tuning \( \tilde{L} \) Implementation

Over the years, several variations of the Chua’s oscillators have been developed [9]. Similarly, master/slave coupling between two Chua’s oscillators for state \( v_1 \) (and \( v_2 \)) is easily achievable with just one resistor and one op-amp (Figure 1). However, measuring and controlling the state \( i_L \) is not as trivial. Therefore variations of inductorless implementations of Chua’s oscillators have been developed [9]. This paper implements the adaptive controller (5) which tunes the parameter \( \tilde{L} \) to \( L \). The measurement of \( i_L \) and \( \tilde{i}_L \) along with the ability to tune \( \tilde{L} \) is possible by using inductor-gyrators made up of CFOAs. Refer to our parallel experimental work [15] for detailed explanation of the circuitry required for this task.

### 5 SPICE and MATLAB Simulation Results

#### 5.1 SPICE Simulation Results

SPICE simulations are done to mimic an experimental scenario to examine the influence of unmodeled parasitic effects on the physical system that are not amenable to examination using the ideal circuit equations such as (1),
(3), and (5). This simulation strategy can be an integral step in designing complex chaotic experiments. Hence, we develop a SPICE simulation model (see Figure 2) containing the various non-ideal behaviors of components such that the simulation model can closely represent a plausible experiment. This includes extracting the signals $i_L$ and $i_{\tilde{L}}$ by measuring the voltages at nodes $v_q$ and $v_{hq}$ in the SPICE simulation (see Figure 2) as opposed to directly extracting $i_L$ ($v_q = i_L R_{1m}$) and $i_{\tilde{L}}$ ($v_{hq} = i_{\tilde{L}} R_{1m}$). The SPICE simulator TINA-TI V9 [16] is chosen because of the capability of its numerical solver.

---

**Fig. 2.** Schematic of master/slave Chua’s oscillator as constructed in the TINA-TI SPICE simulation software.
to optimize its tolerance parameters for convergence. As shown in Figure 2, we used three distinct integrated circuits (ICs), the AD633, the AD844, and the TL082. High fidelity SPICE Macro-Models [1, 2, 17] of each IC are used in the SPICE simulation. Similarly, the JFET used, the 2N3819, is modeled in TINA-TI V9 using the Skickman-Hodges model with specific parameters for the 2N3819 already embedded in the software. Simulation is run using the order 2 trapezoidal integration method. Two initial conditions are set to -6V and 6V at nodes $v_2$ and $\tilde{v}_2$, respectively. The AD633 input terminal $Z$ has a direct $-5$ mV source connected to it for the purpose of compensating for the internal DC offset of the AD633.

The simulation uses the ideal values of the passive components for the master Chua’s oscillator as shown in Table 1. In addition, values of passive components in the slave Chua’s oscillator and adaptive controller are increased by their respective tolerances as indicated in Table 1. These tolerances are selected based on commercially available components.

<table>
<thead>
<tr>
<th>Master Chua’s Oscillator</th>
<th>Adaptive Controller</th>
<th>Slave Chua’s Oscillator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_1 = 22 , k\Omega$</td>
<td>$R_{u_1} = 500 , \Omega$ 1%</td>
<td>$R_1 = 22 , k\Omega$ 0.1%</td>
</tr>
<tr>
<td>$R_2 = 22 , k\Omega$</td>
<td>$R_f = 1 , k\Omega$ 0.1%</td>
<td>$R_2 = 22 , k\Omega$ 0.1%</td>
</tr>
<tr>
<td>$R_3 = 3.3 , k\Omega$</td>
<td>$C_1 = 18 , nF$ 3%</td>
<td>$R_3 = 3.3 , k\Omega$ 0.1%</td>
</tr>
<tr>
<td>$R_4 = 220 , \Omega$</td>
<td>$R_t = 1.1 , k\Omega$ 0.1%</td>
<td>$R_4 = 220 , \Omega$ 0.1%</td>
</tr>
<tr>
<td>$R_5 = 220 , \Omega$</td>
<td>$R_f = 220 , \Omega$ 0.1%</td>
<td>$R_5 = 220 , \Omega$ 0.1%</td>
</tr>
<tr>
<td>$R_6 = 2.2 , k\Omega$</td>
<td>$R_t = 1.7 , k\Omega$ 0.1%</td>
<td>$R_6 = 2.2 , k\Omega$ 0.1%</td>
</tr>
<tr>
<td>$R = 1.7 , k\Omega$</td>
<td>$C_1 = 10 , nF$</td>
<td>$R = 1.7 , k\Omega$ 0.1%</td>
</tr>
<tr>
<td>$C_1 = 10 , nF$</td>
<td>$C_1 = 18 , nF$ 3%</td>
<td>$C_2 = 100 , nF$ 1%</td>
</tr>
<tr>
<td>$C_2 = 100 , nF$</td>
<td>$C_2 = 100 , nF$ 1%</td>
<td>$C = 18 , nF$ 3%</td>
</tr>
<tr>
<td>$R_0 = 200 , \Omega$</td>
<td>$R_0 = 200 , \Omega$ 0.1%</td>
<td>$R_0 = 200 , \Omega$ 0.1%</td>
</tr>
<tr>
<td>$R_{1m} = 1 , k\Omega$</td>
<td>$R_{1m} = 1 , k\Omega$ 0.1%</td>
<td>$R_{1m} = 1 , k\Omega$ 0.1%</td>
</tr>
<tr>
<td>$R_{2m} = 2.25 , k\Omega$</td>
<td>$R_{2m} = 2.25 , k\Omega$ 0.1%</td>
<td>$R_{2m} = 2.25 , k\Omega$ 0.1%</td>
</tr>
<tr>
<td>$R_{3m} = 1 , k\Omega$</td>
<td>$R_{3m} = 1 , k\Omega$ 0.1%</td>
<td>$R_{3m} = 1 , k\Omega$ 0.1%</td>
</tr>
</tbody>
</table>
| $R_{DS} = 1 \, k\Omega$| TR = 2N3819 | $TR = 2N3819$

To quantify how well the master/slave system synchronizes, we use the 2-norm of $[e_{v_1}, e_{v_2}, e_{i_L}]^T$ as our measure, ($e_{\text{norm}} = \| [e_{v_1}, e_{v_2}, e_{i_L}]^T \|$), and observe its evolution over time. Using the signals $i_L$ and $\tilde{v}_2$ we estimate $\tilde{L}$ and $\tilde{R}_0$ ($\tilde{L}_{\text{est}}$, $\tilde{R}_{0\text{est}}$) with a sliding window least square algorithm. Similarly, using signals $i_L$ and $\tilde{v}_2$ we estimate $L$ and $R_0$ ($L_{\text{est}}$, $R_{0\text{est}}$). Comparing these estimates allows us to examine how well $\tilde{L}$ converges to $L$. The transient experimental data is displayed in Figure 3, divided into parts (a)–(e). Switch SW1 is opened at $t = 0.025 s$ which initiates adaptation. Each point on Figure 3(c) represents a least square estimate of a window of 50 samples and the x-axis indicates the time when the leading sample is taken. Figure 3(d) and Figure 3(e) re-plot the last 10 ms of Figure 3(b) and Figure 3(c), respectively, to better visualize the
steady-state results. The average of each signal (except $V_c$) in sections (d) and (e) is listed in Table 2.

Table 2. SPICE simulation: Adapting for $\tilde{L}$ with tolerances.

<table>
<thead>
<tr>
<th>$R_0 = 200 , \Omega$</th>
<th>$R_{\text{est}} = 202.89 , \Omega$ (average)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tilde{R}_0 = 200.2 , \Omega$</td>
<td>$\tilde{R}_{\text{est}} = 202.84 , \Omega$ (average)</td>
</tr>
<tr>
<td>$L = 40.5 , \text{mH}$ (see (21) [15])</td>
<td>$L_{\text{est}} = 45.4 , \text{mH}$ (average)</td>
</tr>
<tr>
<td>$\epsilon_{\text{norm}} = 1.8 \times 10^{-3}$ (average)</td>
<td>$\tilde{L}_{\text{est}} = 45.3 , \text{mH}$ (average)</td>
</tr>
</tbody>
</table>

Fig. 3. SPICE simulation: Adapting for $\tilde{L}$ with tolerances.
5.2 MATLAB Simulation Results

MATLAB-Simulink simulations are run to examine the performance of the adaptive control laws derived in Section 3 as a function of the behavior of the master Chua’s oscillator which changes from chaotic to equilibrium behavior. Simulations are run 1,000 times for 1,000 different values of $C_1$ ranging from 10 nF to 13 nF. With each change in the $C_1$ value, the simulation result for the master Chua’s attractor also changes. To illustrate the change in the master Chua’s attractor with the change in the value of $C_1$, Figure 4 provides the bifurcation diagram for the master Chua’s oscillator for the 1,000 values of $C_1$. To capture the impact of component tolerances the slave Chua’s oscillator parameters are increased by 0.1% (not including $\tilde{C}_1$, which is set to $C_1$).

All simulations are set up as follows: simulations are run by using the Runge-Kutta 4th order numerical solver with a fixed step-size of 10 microseconds for a simulation time of two seconds. The initial conditions are selected to be $v_1(0) = 1$, $v_2(0) = 0$, $i_L(0) = 0$, $\tilde{v}_1(0) = 2$, $\tilde{v}_2(0) = 0$, and $\tilde{i}_L(0) = 0$. Since it takes time for the master Chua’s oscillator to evolve from the initial condition to reach the attractor corresponding to the chosen $C_1$ value, the parameter update law is activated only after 0.5 seconds into the simulation. The parameters used in simulations are listed in Table 3. Figure 4 shows the results for the MATLAB simulation. Figure 4 uses three measures to examine the performance of the adaptive controller. The first performance measure is the error $e_\rho(t = 2)$, that is the parameter error after two seconds of simulation time averaged over the last 10 ms of simulation. The second performance measure is $e_{\text{norm}}(t = 2)$, that is the norm of the error state vector after two seconds of simulation time averaged over the last 10 ms of simulation. Finally, the third performance measure is the settling time ($t_{\text{st}}$), that is the time it takes the slave oscillator’s adaptive parameter to reach within 10% of the master’s corresponding fixed parameter.

Table 3. MATLAB simulation parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Equivalent Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G$</td>
<td>$=\frac{1}{1700}$ S</td>
<td>$G = \frac{1}{1700} + \frac{1}{1700000}$ S</td>
</tr>
<tr>
<td>$R_0$</td>
<td>$=13$ $\Omega$</td>
<td>$\tilde{R}_0 = 13.013$ $\Omega$</td>
</tr>
<tr>
<td>$G_a$</td>
<td>$=-0.40909$ $\text{mS}$</td>
<td>$\tilde{G}_a = -0.40949909$ $\text{mS}$</td>
</tr>
<tr>
<td>$G_b$</td>
<td>$=-0.75758$ $\text{mS}$</td>
<td>$\tilde{G}_b = -0.75833758$ $\text{mS}$</td>
</tr>
<tr>
<td>$E_1$</td>
<td>$=1.1739$ $\text{V}$</td>
<td>$\tilde{E}_1 = 1.1750739$ $\text{V}$</td>
</tr>
<tr>
<td>$G_{u_1}$</td>
<td>$=1/500$ $\text{S}$</td>
<td>$\tilde{G}_{u_1} = 1/500 + 1/500000$ $\text{S}$</td>
</tr>
<tr>
<td>$C_2$</td>
<td>$=100$ $\text{nF}$</td>
<td>$\tilde{C}_2 = 100.1$ $\text{nF}$</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>$=5 \times 10^{-7}$</td>
<td>$L = 18$ $\text{mH}$</td>
</tr>
<tr>
<td>$\tilde{R}_0$</td>
<td>$=13.013$ $\Omega$</td>
<td>$\tilde{L}(0) = 10$ $\text{mH}$</td>
</tr>
</tbody>
</table>

5.3 Discussion

We first comment on the overall performance of the SPICE simulation performed in Section 5.1 by observing Figures 3(b) and 3(c). In the macro scale plot, once the adaptive controller is activated at $t = 0.025$ s, the measure $e_{\text{norm}}$ approaches zero and the estimates of the slave oscillator parameters ($\tilde{R}_0$ and $\tilde{L}$) approach the corresponding parameter values of the master oscillator. However, in Figure 3(c), estimated values of $R_0$ and $\tilde{R}_0$ undergo change despite the fact that $R_0$ is a fixed parameter and the parameter update law is only
Supposed to change the parameter value $\tilde{L}$. This indicates that the inductor-gyrator is not a pure inductor but only a good-enough model for this system to operate within certain tolerances. Next, we examine Figures 3(d) and 3(e) which show the last 10ms of Figures 3(b) and 3(c), respectively. The state errors between the master and slave Chua’s oscillator still exist and the parameters $L$ and $\tilde{L}$ do not perfectly match, with a 0.1mH difference on average (Table 2). This mismatch is attributed to component tolerances. In a simulation study of adaptive synchronization of Chua’s oscillators with a mismatched parameter, [12] similarly observed that the adaptive parameter does not converge to the desired value. Repeating the SPICE simulation without including competent tolerances (see Table 4 and Figure 5), it is seen by averaging the last 10 ms of the 40 ms simulation that there is no difference between $L_{\text{est}}$ and $\tilde{L}_{\text{est}}$.

Next, we comment on our MATLAB simulation results (Figure 4) that illustrate how the adaptive controller performs depending on the behavior of the master Chua’s oscillator. Note that adaptation of parameter $\tilde{L}$ occurs regardless of the system being chaotic or a simple oscillator. The adaptive controller stops working only when the master Chua’s oscillator is in steady state. A close examination of Figure 4 reveals a large spike in $e_{\text{norm}}$ at around $C_1 = 12.32$ nF. This spike is due to the fact that in this small range of $C_1$ the Chua’s oscillator is approaching equilibrium very slowly in which the 2 second simulation time is not enough for the master Chua’s oscillator to reach its steady state behavior. The only time $e_{\text{norm}}$ reaches close to zero is when the Chua’s attractor is in equilibrium, which is when $C_1$ goes above 12.33 nF. At equilibrium, the energy storing components no longer have a long term effect on the system and the

Fig. 4. MATLAB Simulation: Adapting for $\tilde{L}$ with tolerances.
inductor functionally behaves as a short and the capacitors behave as open. In this mode, the adaptive parameters do not converge to any particular value but stay the same. Additional MATLAB simulations conducted with ideal parameter values show that the errors decrease by several orders of magnitude (see Figure 6).

Table 4. SPICE simulation: Adapting for $\tilde{L}$ without tolerances.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Estimated Value</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_0$</td>
<td>200 $\Omega$</td>
<td>$R_{est}$</td>
<td>202.42</td>
</tr>
<tr>
<td>$\tilde{R}_0$</td>
<td>200 $\Omega$</td>
<td>$\tilde{R}_{est}$</td>
<td>202.46</td>
</tr>
<tr>
<td>$L$</td>
<td>40.5 mH (see (21) [15])</td>
<td>$L_{est}$</td>
<td>45.4 mH</td>
</tr>
<tr>
<td>$e_{norm}$</td>
<td>$1.6 \times 10^{-3}$ (average)</td>
<td>$\tilde{L}_{est}$</td>
<td>45.4 mH</td>
</tr>
</tbody>
</table>

---

Fig. 5. SPICE simulation: Adapting for $\tilde{L}$ without tolerances.
6 Conclusion

In this paper we presented an adaptive controller that is designed to match a parameter ($L$) in two Chua’s oscillators with the presence of PE. We implemented the adaptive controller using analog circuitry in a high-fidelity SPICE simulation while incorporating reasonable electrical component tolerances. Furthermore, we tested our adaptive controllers over many conditions of the Chua’s oscillator using MATLAB simulations. Our results show that the adaptive controller achieves parameter matching with a certain degree of error due to tolerance mismatch of the master and slave Chua’s oscillator. In addition, the adaptive controller performs not only when the master Chua’s oscillator is in the chaotic mode but also when the system is a simple oscillator (and does not fulfill the qualities of PE).

Acknowledgements

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References

Chaos in hydrodynamic models of pulsating BL Her-type stars

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Abstract. We present hydrodynamic models of pulsating BL Her-type stars that show a wealth of dynamical behaviours characteristic for deterministic chaos. Interesting phenomena detected in our models include period doubling and intermittent routes to chaos, periodic windows within chaotic domain, type I and type III intermittency, interior crisis bifurcation and others. Before we describe the models, we briefly review the current knowledge about type II Cepheids, a group of radially pulsating stars to which BL Her class belongs, and the methods used to model such stars.

Keywords: astrophysics, pulsating stars, type II Cepheids, chaos, intermittency.

1 Type II Cepheids

Type II Cepheids are low-mass ($M \approx 0.5 - 0.7\, M_\odot$), giant stars pulsating radially with periods from one to several tenths of days (see e.g. Wallerstein\cite{1} or Soszynski et al.\cite{2}). In the H-R diagram, a plot of absolute luminosity ($L$) vs. the effective temperature ($T_{\text{eff}}$), these stars are located in the cool and luminous part, within the instability strip (IS), in which pulsations are driven with the opacity (kappa) mechanism (e.g. Cox\cite{3}). Type II Cepheids are divided into three classes: BL Her stars, with periods between 1 and 4 days, W Vir stars with periods between 4 and 20 days and RV Tau stars with periods above 20 days. The borderline between BL Her and W Vir stars is somewhat arbitrary (see Soszynski et al.\cite{2}). RV Tau stars, on the other hand, are distinguished by period-doubled pulsation which starts to appear at periods above 20 days. Recent studies show however, that effect can appear also at shorter periods, in particular the W Vir star, a prototype of the W Vir class, shows the effect (Templeton & Henden\cite{4}). In addition, the period doubling effect was discovered in one BL Her star with period $\approx 2.4$ days (Smolec et al\cite{5}). The possible existence of period doubled BL Her stars was predicted by Buchler & Moskalik\cite{6} 20 years earlier, based on hydrodynamic models.

Type II Cepheids are at advanced evolutionary stages (see Wallerstein\cite{1}, Gingold\cite{7}). The division into three classes is believed to reflect different evolutionary stages of the stars. After hydrogen is depleted in the core, the star climbs up the Red Giant Branch (RGB) increasing its luminosity at nearly

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constant effective temperature. After the helium is ignited in the degenerate core, the progenitors of type II Cepheids arrive at the blue side of the Zero-Age Horizontal Branch (ZAHB), steadily burning helium in the center. They evolve redward, towards the Asymptotic Giant Branch (AGB) and, as they cross the instability strip, they pulsate as BL Her variables. As helium is depleted in the core, its burning continues, along with the hydrogen burning, in the shells surrounding the carbon/oxygen core. The star, now climbing up the AGB, may loop back into the IS due to instabilities in the shell burning, becoming a W Vir-type variable. Finally, as the star leaves the AGB on the way to the white dwarf sequence, it crosses the IS for the last time, pulsating as RV Tau-type variable.

In majority of cases, the least luminous, shortest period BL Her stars are very regular pulsators, with repeatedly stable cycle-to-cycle variation. As luminosity increases the light variation becomes less regular. Irregular amplitude and period variation is frequently observed in W Vir stars. Strong irregularities on top of period-doubled pulsations are common in RV Tau stars. The behaviour is more pronounced in longer period stars. Closely related to RV Tau stars, even more luminous and longer period semi-regular and Mira-type pulsators, show very strong irregular cycle-to-cycle variation, without evident period doubling. Deterministic chaos was detected in two RV Tau-type stars and in a few semi-regular and one Mira-type variable, for which long (at least 30 years) and good quality observations allowed a rigorous analysis (Buchler et al.[8], Kolláth et al.[9], Buchler, Kolláth & Cadmus,[10], Kiss & Szatmáry[11]). Hydrodynamic models of type II Cepheids indicate that indeed, as pulsation period increases a period-doubling route leads to deterministic chaos (Buchler & Kovács[12], Kovács & Buchler[13]). We note however, that no period-4 (or other than period-2) pulsating star is known to date.

2 Hydrodynamic models of BL Her stars

For more than 50 years now, large amplitude radially pulsating stars are investigated with the help of one dimension pulsation hydrocodes. The first calculations were purely radiative, neglecting the energy transfer by convection. Nowadays, simple 1D recipes for time-dependent turbulent convection are used. In our study of BL Her models we used our nonlinear code (Smolec & Moskalik[14]) implementing the Kuhfuß[15] one-equation, turbulent convection recipe. Equations we solve are momentum, internal and turbulent energy equations:

\[
\frac{du}{dt} = -\frac{1}{\rho} \frac{\partial}{\partial r} \left( p + p_t \right) + U_a - \frac{GM_r}{r^2},
\]

\[
\frac{dE}{dt} + p \frac{dV}{dt} = -\frac{1}{\rho} \frac{\partial}{\partial r} \left[ r^2 \left( F_r + F_c \right) \right] - C,
\]

\[
\frac{de_t}{dt} + p_t \frac{dV}{dt} = -\frac{1}{\rho} \frac{\partial (r^2 F_t)}{\partial r} + E_a + C.
\]
with
\[ u = \frac{dr}{dt} \]  \hspace{1cm} (4)

Above, \( u \) is fluid velocity, \( M_r \) is mass enclosed in radius \( r \), \( V \) is specific volume (inverse of specific density, \( V = 1/\rho \)), \( p \) and \( E \) are pressure and energy of the gas. \( F_r \), \( F_c \) and \( F_t \) are radiative, convective and turbulent fluxes, respectively. Radiative flux is computed assuming diffusion approximation and radiation pressure and radiation energy are included in \( p \) and \( E \). Turbulent energy, \( e_t \), is computed according to model of Kuhfuß. \( p_t \) is turbulent pressure and \( U_q \) and \( E_q \) are viscous momentum and energy transfer rates. The internal and turbulent energy equations are coupled through the term \( C \):
\[ C = S - D - D_r , \] \hspace{1cm} (5)

with source (or driving) function, \( S \), describing the rate of turbulent energy generation/damping through the buoyant forces, \( D \) modelling the decay of turbulent energy through the turbulent cascade and \( D_r \) describing the rate at which turbulent energy is transformed to the internal energy, through the radiative cooling of the convective eddies. The model contains eight parameters, values of which are calibrated using observational constraints. The reader is referred to Smolec & Moskalik\[14\] for further details.

To construct a model of pulsating star we first solve the static version of equations (1)–(3). The model is divided typically into 150–200 lagrangian mass shells extending down to a fixed temperature of a few million Kelvin. It is not necessary to model the deeper stellar interior as pulsation amplitudes are negligibly small there. The equilibrium model is subject to linear stability analysis, which yields periods and linear eigenvectors of the pulsation modes. All known type II Cepheids pulsate in the lowest frequency fundamental mode. The static model is perturbed with the scaled velocity eigenvector and equations (1)–(4) are integrated in time till steady pulsation state is reached. In majority of the studies focused on classical pulsators, RR Lyrae stars or classical Cepheids, the model converges to a limit cycle – full amplitude, single-periodic pulsation. In our recent studies of type-II Cepheids of BL Her type a much more interesting solutions were found, including period doubled pulsation, nicely reproducing the observations of the only BL Her star showing the effect (Smolec et al.[5]) and periodic and quasiperiodic modulation of pulsation (Smolec & Moskalik\[16\]). In this contribution we discuss an even more complex behaviour we found in BL Her type models with decreased eddy-viscous dissipation – deterministic chaos.

We discuss a single sequence of BL Her-type models, with the same mass \( (M = 0.55M_\odot) \), the same luminosity \( (L = 136L_\odot) \), the same chemical composition and varying effective temperature, which is a control parameter in the following. The models cover a 170 K stripe in the H-R diagram and were computed with the maximum step in effective temperature of 1 K, decreased to 0.1 K in the most interesting domains. The models were integrated typically for 10 000 pulsation cycles (up to 50 000 for few cases) and radius variation, in particular the values of maximum radius, were analysed in detail. Smolec & Moskalik\[17\] present a detailed description and analysis of these models.
3 Chaotic phenomena in BL Her models – a showcase

Figure 1 presents a bifurcation diagram for the computed BL Her models. It is a stack of grey-scaled histograms. For each effective temperature we computed the probability with which the maximum radii fall into 120 bins into which the range of maximum radius variation in the models was divided. In the bottom part of Fig. 1 values of the largest Lyapunov exponents, computed using the algorithm of Rosenstein, Collins & De Luca[18], are plotted. They are positive, with typical values between 0.15 d^{-1} and 0.20 d^{-1}, dropping significantly at the edges of the chaotic bands. Period doubling route to chaos is evident both from the cool and the hot side of the computation domain. Period doubling cascade up to period-16 (on the hot side) is detected in our model grid. The length of period-2k domain, d_{2k}, decreases as k increases. The ratios d_{2k}/d_{4k} are estimated to d_{2}/d_{4} = (3.6 \pm 0.4) K and d_{4}/d_{8} = (5 \pm 2.5) K (on the hot side), and d_{2}/d_{4} = (3.5 \pm 0.9) K (on the cool side), and do not differ significantly from the Feigenbaum constant. The chaotic band is split into parts by several windows with periodic variation. The largest, period-3 window, is the most interesting. At its cool side, as effective temperature decreases, an intermittent route to chaos is detected (Pomeau and Manneville[19]). On its hot side, the period doubling route leads to three chaotic bands which merge into one in an interior crisis bifurcation (Grebogi, Ott and Yorke[20]). Below we highlight these and other interesting phenomena we detect in our models.

![Bifurcation diagram](image)

**Fig. 1.** Bifurcation diagram for the computed hydrodynamic models (top) and variation of the largest Lyapunov exponent (bottom).

- **Chaotic models.** In Fig. 2 we display first return maps for two hydrodynamic models followed for 50 000 pulsation cycles. Complex and likely fractal structure of the attractor is well visible.
- **Periodic windows.** We detect seven windows with periodic behaviour. Three of the windows, with period-6 (at T_{eff} = 6371 K), period-5 (at T_{eff} = 6383 K) and period-6 (at T_{eff} = 6479 K) behaviour, are less than 2 K wide.
Return map for the model located in first of these windows is displayed in Fig. 3 (left). In a window extending between 6397 K and 6400 K period-7 and, after a period doubling bifurcation, period-14 behaviours are detected. In a window extending between 6363 K and 6366 K complex scenario is observed – see return map in Fig. 3 (right), including type-III intermittency discussed below. The two largest windows, period-3 (6421 K–6438 K) and period-6 (6459 K–6468 K) windows, show a rich internal structure, with period-doubling and intermittent routes to chaos. These are also discussed in more detail below.

Fig. 2. First return maps for two models showing chaotic variability.

Fig. 3. First return map for a period-6 model (left) and four models from period-9 window. In both cases first return maps for directly neighbouring, slightly cooler, chaotic models are plotted with grey dots, for a reference.
• **Type III intermittency.** The effect is clearly observed in one model from period-9 window \( (T_{\text{eff}} = 6365 \, \text{K}) \) In a return map (Fig. 3, right) 9 bands are clearly visible, while inspection of maximum radii (Fig. 4) clearly reveals type-III intermittency: switching between period-9 and period-18 behaviour (see Pomeau and Manneville[19]).

![Fig. 4. Type III intermittency in a model with \( T_{\text{eff}} = 6365.0 \, \text{K} \).](image)

• **Type I intermittency.** The effect is best visible at the cool edge of the largest, period-3 window, at which, as effective temperature of the models is decreased, the intermittent route to chaos is evident. In Fig. 5 the maximum radii are plotted vs. the pulsation cycle number for two models with 6420.9 K and 6420.7 K. We note that a slightly hotter model (6421 K) displays a strictly periodic, period-3 behaviour. As effective temperature is decreased, period-3 cycle losses its stability (tangent bifurcation) and type I intermittency is observed with the stages of almost periodic behaviour rapidly shrinking with the growing distance from the bifurcation point.

• **Interior crisis and crisis induced intermittency.** These phenomena are present on the hot side of the period-3 window. There, at \( T_{\text{eff}} \approx 6435 \, \text{K} \), a period doubling cascade forms three separated chaotic bands. As effective temperature is increased, these three bands hit the unstable period-3 cycle created in the tangent bifurcation at the cool edge of the period-3 window, expand, and merge into one chaotic band \( (T_{\text{eff}} \approx 6438 \, \text{K}) \). A crisis induced intermittency is well visible in slightly hotter models and is illustrated in Fig. 6.

• **Remerging Feigenbaum tree.** The period-3 and period-6 windows are tightly connected, as is well visible in the bifurcation diagram (Fig. 1), and form a period-3 bubble or remerging Feigenbaum tree (Bier & Bountis[21]). The scenarios at the cool and at the hot side of the chaotic band separating these two windows are mutual mirror images. In addition the three chaotic bands that are formed in the two windows (as temperature is increased within period-3 window, and as temperature is decreased in period-6 window) do not disappear as they merge into one band in the crisis bifurcation.
Fig. 5. Type I intermittency in a model with $T_{\text{eff}} = 6420.9$ K (top) and in a model 0.2 K cooler (bottom).

Fig. 6. Crisis induced intermittency in a model with $T_{\text{eff}} = 6438.4$ K.

They sustain their identity and smoothly merge within the chaotic domain (between 6438 K and 6459 K) as dark grey bands in Fig. 1 indicate.

4 Discussion

Most of the chaotic phenomena detected in the models were not yet detected in pulsating stars. In BL Her stars only period doubling effect was found in one star. Nevertheless chaotic dynamics is present in more luminous type II Cepheids of RV Tau type and in semi-regular and Mira-type variables. Based on our models we expect, that the wealth of dynamical behaviours well known in
classical dynamic systems, like Lorenz or Rössler systems, may also be present in pulsating stars. Detection of these effects is difficult however, as long, regular and precise monitoring of stellar variability is necessary. With the growing amount of high quality data from massive sky surveys, like Optical Gravitational Lensing Experiment (Udalski et al.[22]), we hope that discovery of the reported effects, like intermittency or period-$k$ pulsation (with $k$ other than 2), is only a matter of time.

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References


Energy and Frequency Location as Criteria for Chaotic Encryption on Unidimensional Signals


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Abstract. In this paper the encryption, transmission and recovery of a confidential message using chaotic signals is presented. The communication process is made in a two-channel communication system with multi-user modality. Here, the authors suggest the consideration of two criteria to choose the suitable chaotic signal, so that, the security level of the encrypted message would be improved. The criteria consider the characteristics of the chaotic signals, such as energy and frequency location. To achieve this objective, the synchronization of chaotic systems is needed, for this reason, these systems are arranged in topologies of complex networks and synchronized using the Complex Systems Theory.

Keywords: Private communications, Chaotic encryption, Chaotic oscillator, Synchronization, Complex network.

1 Introduction

Driven by the idea of hiding and restricting access to certain information, mankind has developed increasingly complex ways to carry out the encryption of data; among the methodologies that have been explored to hide information, the chaotic encryption is one of the main alternatives.

Chaotic oscillators have received lots of attention in the last decade because of their potential application in private communications. These systems have attracted the interest of the researchers who have studied and implemented these extensively in the field of communications [1].

Particularly, in this paper, chaos generators exhibit scrolls chaotic attractors, these models are capable of generating scrolls along any of its state variables, these nonlinear dynamical systems belong to the family of grid-scroll attractors in 1-D, 2-D and 3-D.

A new family of n-scroll attractors [1,2] are used as generators of chaotic signals which for simplicity will be called Genesio & Tesi 3-D (G&T 3-D) chaotic oscillators as this model is a generalization of the original model that R. Genesio and A. Tesi proposed in 1992 [1–3].

The chaotic communications is an area that has been active in the last decade, this is because the non-periodicity and apparent randomness of chaotic
signals are the main benefits observed [4], nevertheless, the encryption process lacks a selection criteria to choose the suitable chaotic signal to encrypt, this in the sense of satisfying the message requirements, i.e., the correct masking in time and frequency domain.

In this work, the selection criteria of chaotic signal based on the energy characteristics of the signal is proposed. Finally, to reach the purpose of this research, the synchronization of chaotic oscillators is needed, for this reason, some results of synchronization of G&T 3-D chaotic oscillators arranged in topologies of complex networks are presented.

This paper is organized as follows: In Section II a brief review on synchronization of complex dynamical networks is given. In Section III, the problem of synchronization in N-coupled chaotic systems in complex networks is exposed as well as the basic model of multi-scroll attractor G&T 3-D system that is used as chaos generator; the corresponding synchronization results are provided also in this section. In Section IV, the criteria proposed to choose the chaotic signal are shown and explained as well as the results of the encryption, transmission and recovery of a confidential message test. In Section V some conclusions are given.

2 Complex networks

A complex network is defined as an interconnected set of nodes, where each node is a fundamental unit, with its dynamics depending of the nature of the network. Each node is defined as follows:

\[ \dot{x}_i = f(x_i) + u_i, \quad x_i(0) = c_i, \quad i = 1, 2, \ldots, N, \]

where \( x_i = [x_{i1} \ x_{i2} \ \ldots \ x_{in}] \in \mathbb{R}^n \) are the state variables of the node \( i \), \( c_i \in \mathbb{R} \) are the initial conditions and \( u_i \in \mathbb{R}^n \) establishes the synchronization between two or more nodes and is defined as follows [5]

\[ u_i = c \sum_{j=1}^{N} a_{ij} \Gamma x_j, \quad i = 1, 2, \ldots, N, \]

the constant \( c \) positive definite represents the coupling strength and \( \Gamma \) is a constant matrix linking coupled state variables. In this matrix, two nodes are linked through their \( i \)th state variables. Assume that \( \Gamma = \text{diag}(r_1, r_2, \ldots, r_n) \) is a diagonal matrix with \( r_i = 1 \) for a particular \( i \) and \( r_j = 0 \) for \( j \neq i \).

The matrix \( A = (a_{ij}) \in \mathbb{R}^{N \times N} \) is the coupling matrix which shows a connection between node \( i \) and \( j \), if this is the case, then \( a_{ij} = 1 \), otherwise \( a_{ij} = 0 \) for \( i \neq j \). The diagonal elements of \( A \) are defined as

\[ a_{ii} = - \sum_{j=1, j \neq i}^{N} a_{ij} = - \sum_{j=1, j \neq i}^{N} a_{ji} \quad i = 1, 2, \ldots, N. \]

The dynamical complex network (1) and (2) is said to achieve synchronization if \( x_1(t) = x_2(t) = \ldots = x_n(t) \). \( t \to \infty \). A network with \( N \) identical multi-scroll attractors G&T 3-D as nodes is considered.
3 Synchronization of \( N \) multi-scroll attractor Genesio & Tesi 3-D via coupling matrix

In this section, synchronization of complex networks constituted of \( N \)-coupled multi-scroll attractor G&T 3-D is achieved. First, it is shown the set of equations that describes the multi-scroll attractors G&T 3-D; then, necessary data to achieve synchronization is provided; finally, at the end of the section synchronization results are shown.

Multi-scroll attractor G&T 3-D chaotic oscillator is described by

\[
\begin{align*}
\dot{x} &= y - f_1(y), \\
\dot{y} &= z - f_1(z), \\
\dot{z} &= -ax - ay - az + af_3(x),
\end{align*}
\]

where

\[
\begin{align*}
f_1(y) &= \sum_{i=1}^{M_y} g_{1,2i+1}(y) + \sum_{i=1}^{N_y} g_{1,2i+1}(y), \\
f_1(z) &= \sum_{i=1}^{M_z} g_{1,2i+1}(z) + \sum_{i=1}^{N_z} g_{1,2i+1}(z), \\
f_3(x) &= \sum_{i=1}^{k-1} \gamma g_{ni}(x),
\end{align*}
\]

\[
g_\theta(\cdot) = \begin{cases} 
1, & \cdot \geq \theta, \theta > 0, \\
0, & \cdot < \theta, \theta > 0, \\
0, & \cdot \geq \theta, \theta < 0, \\
-1, & \cdot < \theta, \theta < 0,
\end{cases}
\]

and \( \gamma = \max\{\gamma_{ij}\} = \max\{u_{ij}^{eq,y} + u_{ij}^{eq,z}\} \). Here, \( x, y, z \) are equilibria points, \( a = 0.8, u^{eq,y} \) and \( u^{eq,z} \) are the vectors for the \( y \) and \( z \) variables related to the equilibrium points, the Eq. (8) is the core function \([2]\). The equilibrium points satisfy \( x + y + z = f_3(x), y = f_1(y) \) and \( z = f_1(z) \) where the points for the \( y, z \) variables are given by

\[
\begin{align*}
u^{eq,y} &= \{-M_y, \ldots, -1, 0, 1, \ldots, N_y\}, \\
u^{eq,z} &= \{-M_z, \ldots, -1, 0, 1, \ldots, N_z\}.
\end{align*}
\]

Synchronization of a complex networks: A complex network of identical multi-scroll attractor G&T 3-D is synchronized. The coupled network topology is illustrated in Fig. 1, where every oscillator is described by Eqs. (4)-(8); considering a synchronization scheme of \( N \)-coupled multi-scroll attractor G&T 3-D chaotic systems, the coupling matrix corresponding to the displayed topology is obtained because of its size (17 \( \times \) 17) which is obtained as explained in the previous section, all its eigenvalues are 0 = \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \ldots \geq \lambda_{17} \).

The Gamma matrix is defined as \( \Gamma = \text{diag}(1, 0, 0) \), this means that the synchronization is achieved by the first state variable. According to Eq. (1), the control laws \( u_{1i} \) for \( i = 1, \ldots, 17 \) are given by the nonzero \( A \) matrix elements.
The initial conditions for each oscillator are

<table>
<thead>
<tr>
<th>Initial conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1, \ldots, g(0)$</td>
</tr>
<tr>
<td>$y_1, \ldots, g(0)$</td>
</tr>
<tr>
<td>$z_1, \ldots, g(0)$</td>
</tr>
<tr>
<td>$x_{10}, \ldots, 17(0)$</td>
</tr>
<tr>
<td>$y_{10}, \ldots, 17(0)$</td>
</tr>
<tr>
<td>$z_{10}, \ldots, 17(0)$</td>
</tr>
</tbody>
</table>

Table 1. Initial conditions for each oscillator of the complex network in Figure 1.

The coupling strength $c = 10$ was obtained through the stability analysis reported in [6]. With this data, the following synchronization results are obtained: In Fig. 2(a) the chaotic attractor of Eq. (4) with $4 \times 2 \times 2$ scrolls of the complex network is shown; Fig. 2(b) shows only the evolution of the second state variable of each chaotic oscillator, where synchrony can be observed. These chaotic signals will be used in the communication process in the following section. For readers interested in this topic can refer to [10–12] and their references.
4 Selection criteria for the chaotic signal

As above mentioned, chaos generators and chaotic signals have been implemented extensively in the field of private communications [7–9], however, there remains a lack of criteria for choosing the best masking chaotic signal, for this reason, in this section, two criteria of selection are proposed and these are briefly described.

4.1 Criterion 1: selection based in the chaotic signal energy

The first criterion suggests the selection of the chaotic signal based on its energy, using this approach, the higher energy value the better the chaotic signal to encrypt, however, it is not necessary to choose signals with very large indices but only those that meet the requirements of the message to encrypt.

\[
\sum_{n=0}^{N-1} |x_c(n)|^2 \gg \sum_{n=0}^{N-1} |x_m(n)|^2.
\]  \(10\)

Here, \(x_c(n)\) is the chaotic signal and \(x_m(n)\) is the message. The criterion considers a relation between the energy of the message and the chaotic signal, i.e., \(J_1\) will yield how many times the chaotic signal energy exceeds the message energy, with this, \(J_1 \gg 1 \rightarrow \text{good encryption}\).

4.2 Criterion 2: selection based in the chaotic signal energy in the frequency domain

Despite the advantage that means choosing the signal by its level of energy, it is advisable to know its bandwidth, this in order to ensure a good encryption seen from the frequency domain, i.e., considering the frequency range in which the spectrum of the message to encrypt is located. It is very important to know the frequencies where the most energy of the chaotic signal is located to prevent the encrypted message to be retrieved by filtering techniques, this idea is illustrated in Fig. 3.

The second criterion considers the amount of chaotic signal energy in the frequencies where the most energy of the message is located.

\[
\sum_{k=0}^{N-1} \alpha(k)|X_c(k)|^2 \gg \sum_{k=0}^{N-1} \alpha(k)|X_m(k)|^2,
\]  \(11\)

where \(X_c(k)\) are the chaotic signal Fourier coefficients, \(X_m(k)\) are the message Fourier coefficients and \(\alpha(k)\) is the frequency weighting function that selects the frequencies where the message is located. This criterion will give the relation between the chaotic signal energy and the message energy just in a specific frequencies band. Basically, criterion \(J_2\) will show how many times the chaotic signal energy, located in the message bandwidth, is bigger than the message energy; with this \(J_2 \gg 1 \rightarrow \text{good encryption}\). As in the previous case it is recommended to choose the chaotic signal that meets the requirements of the message to encrypt.
4.3 Chaotic encryption

In this section the results of encryption, transmission and recovery of a confidential message are given, also, the criteria above described are considered to choose the chaotic signal from the ones generated in Section 3 as result of synchronization. It is highly recommended to choose the chaotic signal based on both criterions $J_1$ and $J_2$ to prevent a bad encryption.

<table>
<thead>
<tr>
<th>State</th>
<th>$E_c \times 10^7$</th>
<th>$J_1$</th>
<th>$J_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x(t)$</td>
<td>5.5522</td>
<td>265.5872</td>
<td>14.8015</td>
</tr>
<tr>
<td>$y(t)$</td>
<td>0.0724</td>
<td>5.465</td>
<td>1.8041</td>
</tr>
<tr>
<td>$z(t)$</td>
<td>0.0815</td>
<td>3.9023</td>
<td>1.9981</td>
</tr>
</tbody>
</table>

Table 2. Criteria values for the chaotic signal of the synchronization of the complex network in Fig. 1.

The communication diagram is shown in Fig. 4, the transmission process is made in two channels and the recovery in multi-user modality. In Table 2 are shown the resulting values for criteria proposed, where the $\alpha(k)$ function has a unity gain covering 0.025-1 kHz and nule gain at other frequencies.

Here, as shown in the diagram of Fig. 4 the synchronization of transmitter and receptor is made through the first state, according to Table 2, the third state is a good option to encrypt due to the first state has values bigger than necessarily besides that it has been used to synchronize.

In Fig. 5 the resulting signals of the communication process are given. At the top, the message to encrypt $m(t)$ that is a short part of the piano song *Ballad to Adelina*; at the middle, the encrypted message $s(t) = z(t) + m(t)$ that is transmitted by the second channel and finally at the bottom, the retrieved message $m'(t) = s(t) - z'(t)$ for every user.
As we could see, it was accomplished the transmission of a confidential message, where, the encryption was made using a chaotic signal and the recovery through the synchronization of a complex network.

5 Conclusion

In this work the chaotic encryption of an audio signal was made. Authors have proposed two criteria Eqs. (10)-(11) to choose the chaotic signal to encrypt the message in order to improve the security level of the communication process. The criteria consider the energy characteristics of the message and the masking chaotic signals. The resulting indices of each criterion give how good a chaotic signal is to be applied as masking signal. It has been shown that choosing the chaotic signal with indices that cover in a fair way the requirements of the
massage is sufficient to achieve a good encryption. It is important to mention that $J_1$ and $J_2$ do not give local information, i.e., they cannot prevent from bad encryption when the chaotic signal magnitude is smaller than the message magnitude in a specific time interval.

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