Biochemical Reservoir Computing

Hoang Nguyen  
*Portland State University*

Christof Teuscher  
*Portland State University*

Follow this and additional works at: [https://pdxscholar.library.pdx.edu/studentsymposium](https://pdxscholar.library.pdx.edu/studentsymposium)

Part of the Computer Engineering Commons, and the Electrical and Computer Engineering Commons

Let us know how access to this document benefits you.

[https://pdxscholar.library.pdx.edu/studentsymposium/2018/Poster/8](https://pdxscholar.library.pdx.edu/studentsymposium/2018/Poster/8)

This Poster is brought to you for free and open access. It has been accepted for inclusion in Student Research Symposium by an authorized administrator of PDXScholar. Please contact us if we can make this document more accessible: pdxscholar@pdx.edu.
Biochemical Reservoir Computing

Hoang Nguyen – hoang24@pdx.edu
Adviser: Dr. Christof Teuscher
Maseeh College of Engineering and Computer Science
Portland State University

OBJECTIVE
Design and build a reservoir computer (RC) model based on a system of chemical reaction networks (CRNs) that has computational and learning capabilities.

BACKGROUND AND MOTIVATION
Reservoir computing is an emerging machine learning paradigm. Compared to traditional feedforward neural networks, the reservoir can be unstructured and recurrent and only the output layer is trained. Reservoirs can be built with various types of physical components, yet, biochemical building blocks have not been widely used. This project focuses on designing and testing a reservoir computer (RC) based on chemical reaction network (CRN). We simulated high-level CRNs in MATLAB and their complex chemical dynamics were observed over time. A CRN constructed by a network of coupled deoxyribozyme oscillators was chosen for the final RC model. This project thus has the potential to influence biomedical research and genetic disorder treatments.

METHODS
The CRN dynamics inside the reservoir were mathematically modeled by a set of ordinary differential equations (ODEs) shown in (1)

\[
\begin{align*}
\frac{d[M]}{dt} &= \mu[R][G] - [P]\, [M], \\
\frac{d[P]}{dt} &= \mu[R][G] - \frac{3}{2} - \frac{\mu[R][G]}{2} - \frac{P}{2}, \\
\frac{d[G]}{dt} &= \mu[R][G] - \frac{3}{2} - \frac{\mu[R][G]}{2} - \frac{P}{2} \\
\end{align*}
\]

Key parameters:
- \([P] \): concentration of product molecules
- \([M] \): concentration of substrate molecules
- \([G] \): concentration of gate molecules
- \(\mu \): influx rate of the substrate molecules

In the lab, the system of ODEs (1) was solved and simulated with MATLAB ode23s solver using Runge – Kutta method.

RESULTS
In order for the reservoir to start oscillate, the chemistry was unperturbed for 500 seconds, following by a change in the influx rate of at least one substrate. With a single perturbation, this reservoir showed dynamics of an amplifying and attenuating oscillator as shown in figure 2 and 3.

Random perturbations were introduced at different times to produce random oscillations of the product concentrations. In this RC model, substrate(s) were perturbed in every 5 seconds to introduce reservoir inputs. Figure 4 illustrates single perturbations and figure 5 illustrates double perturbations.

ANALYSIS
The computational abilities of this coupled deoxyribozyme RC model were tested by learning the Hamming distance. 1000 different sets of 6-bit inputs were applied to the reservoirs consecutively in 1000 experiments. Table 1 below illustrates the average error of each bit on a sample simulation, together with their targets and actual outputs.

<table>
<thead>
<tr>
<th>Bit index #</th>
<th>Target</th>
<th>Actual output</th>
<th>Average error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>5.299e-04</td>
<td>0.0028</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.9994</td>
<td>0.0025</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>2.146e-10</td>
<td>0.0036</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>2.7559e-05</td>
<td>0.0029</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.9995</td>
<td>0.0034</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>6.4227e-04</td>
<td>0.0031</td>
</tr>
</tbody>
</table>

Table 1: Results of a sample Hamming distance learning performed by the coupled deoxyribozyme oscillators.

CONCLUSION
Here we show that a reservoir computer constructed by a system of coupled deoxyribozyme oscillators is capable of performing computational and learning tasks. From the experiments, the results show that such an RC can successfully learn linearly separable patterns, with an average learning error of 0.0031. Further research will be conducted to minimize the learning error and increase the learning success rate. In addition, DNA strands will be feed into the RC and will be interpreted as the binary bistreams. This model can also be further designed to detect pathogens and genetic mutations.

REFERENCES

ACKNOWLEDGEMENT
This model is based upon work supported by the National Science Foundation under grant no. 1518833. The original RC model of this work was described in “DNA Reservoir Computing: A Novel Molecular Computing Approach” by Goudarzi et al. The authors acknowledge the support of the teuscher lab, the Maseeh College of Engineering and Computer Science, and the University of New Mexico.