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THE THEORY OF COMMUNICATION DYNAMICS Application to Modelling the Valence Shell Orbitals of Periodic Table Elements

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Abstract Atoms are considered basic building blocks of the material world. Computational modelling is a useful technique for studying and predicting natural events. Due to the complexity and wide scale range of particle systems, current computational modelling approaches, including Classical Mechanics, General Relativity, and Quantum Mechanics are separately designed to describe systems at different sizes and precisions. While these disparate models have practical value for discrete, domain-specific problems, lack of consistency between models results in challenges when multi-scale integration and computational scalability is required. In this paper, we proposed a novel theoretical framework, inspired by the communication theory of Shannon, to describe physical reality from a new perspective. We call this approach Communication Dynamics. As an initial demonstration of the relevancy of this model, we represent electron orbital structures of atoms. Our model aims to use a uniformly applicable mathematical formula to describe natural structures at different scales. We believe this information theoretical approach represents a new way to investigate particle-wave duality and opens a pathway to multi-scale model integration between physics and other fields of science. The appendix containing actual calculations is 141-page Wolfram Mathematica file, which can be obtained from SDPS web page.

Keywords: Communication dynamics theory, theory of matter and energy, communication theory, physics, general and special relativity

1. Introduction

The Concept of Communication Channel

In communication theory, a communication channel is defined as the medium through which the information is transmitted from the signal source to the receiver (Shannon and Weaver, 1963). Noise present in the channel alters signals during the transmission. One can model noise as a random computation

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introduced during transmission of the signal. Shannon has mathematically defined the channel and its capacity. A simplified representation of a communication system is shown in Figure 1, with the black box representing the communication channel.

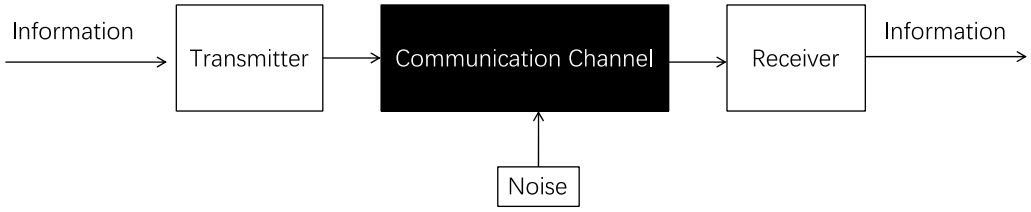


Figure. 1. Shannon's Communication System

The Concept of Communication Dynamics (CD)

The proposed Communication Dynamics Theory has four assumptions:

Assumption 1: The universe (nature) is **anisotropic**.

Assumption 2: The first assumption admits the **second law of thermodynamics** (arrow of time). Time is a description of the evolutionary stage of the universe as a measurement of entropy. The total entropy of the universe is always increasing; therefore, time is not reversible.

Assumption 3: Movement from a low entropy state to a higher entropy state is experienced as a form of **acceleration**. This observed state of acceleration admits the general theory of relativity. Specifically, as the universe accelerates, the speed of time (in terms of clock ticks) can be different in different microsystems. Observers may experience these frequencies as colors (Wilczek, 2015).

Assumption 4: The substance of the universe can be represented as an **accelerating one-dimensional communication system**. All observations, including emergent dimensionality, can be described as a manifestation of this one-dimensional accelerating Spacetime.

In order to construct a model based on these assumptions, several concepts must be defined:

Definition 1 – Computing: A universal form of existence for all natural and artificial systems at every scale of precision. Based on this definition, we use computing to replace conventional physics terms such as interactions, conduction, chemical reactions, entanglement, etc. In Communication Dynamics, a common set of rules governs information exchange. Computing occurs in a domain we will define as Spacetime.

Definition 2 -- Spacetime Point: A Spacetime point $x + it$ is a point in the complex domain. In Communication Dynamics, we assume time is represented by *it* and the space is represented by x.

Definition 3 -- T-Vectors and U-Matrices: In Communication Dynamics we define a new mathematical object to naturally accommodate Spacetime, the Timed Vector (T-Vector). The notion of a T-Vector is an extension of a regular vector definition with the addition of a frequency parameter. A T-Vector is represented by three parameters: magnitude, direction, and frequency. The frequency components of T-Vectors can be represented by Fourier series. We call a special matrix of T-vectors is the U-matrix.

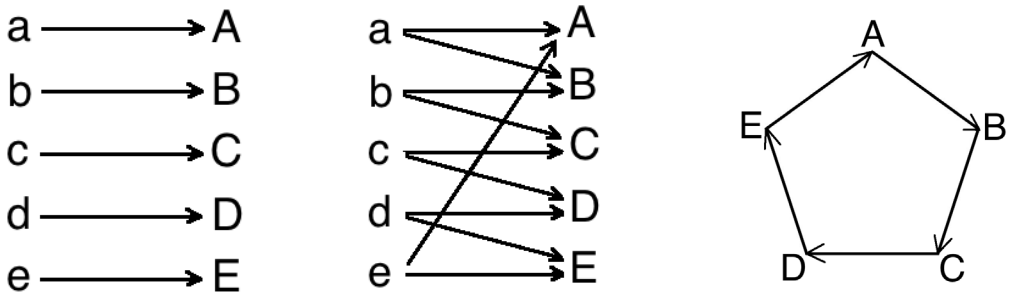
One dimensional Spacetime in Communication Dynamics

Conventional mathematical models for atomic systems treat space and time as separate dimensions. This assumption was expanded by Einstein's general relativity theory by assigning separate clocks at all points (Einstein, 1920). The Communication Dynamics model replaces a "Space + Time" formulation with the concept of Spacetime as a single dimension of chained discrete T-Vectors. Thus, four dimensional Spacetime becomes an emergent property of accelerated, chained discrete T-Vectors. Using the mathematical object of T-Vectors, different scales of systems can be represented with adjustable precision. With modified communication channels, precision can be set as precise as the smallest quantum unit—*h*

(Planck constant) and as large as any defined physical entities such as electrons, atoms, and molecules. The model is scale-invariant and can address the cross-scale integration problem with a uniformly applicable mathematical formulation. Fundamentally, the approach is based on the concept of using a communication theory-based model rather than assuming the existence of space and time as separable elements. Particle based models (i.e. Standard Theory) (Weinberg, 2004) and wave based models (i.e. Electromagnetism) can be represented as "special cases" of the Theory of Communication Dynamics model depending on the values of T-Vector's frequency parameter. In this paper, the Communication Dynamics model has not been fully explored. To demonstrate the capabilities of the model however, we apply the Communication Dynamics Theory to the periodic table of elements, showing a communication channel representation for each element in the periodic table. Specifically, we select the outermost electron orbital as the communication channel. The corresponding physical properties of the orbitals such as energy and radius can also be represented in this model. We plan to introduce other aspects of Communication Dynamics in a series of studies. All inquiries are welcome.

2. Approach

Berge (Berge, 1973) formulated Shannon's noisy channel as an "error content" graph. This "error" in transmission can also be encoded as information that has transferred from (for example) a to B as shown in Figure 2. On the far right, we can represent this transmitted information as an error content (or information content) graph. A regular polygon in the form of an error content graph can be created using Fourier series (Robert, 1994).



A sample "error-free" communication channel (theoretical, left), communication with error (middle) and an error content graph (right).

Figure. 2. Generating Error Content Graphs from Communication Channels

2.1. Electron shells as communication channels

Utilizing Fourier series of polygons as T-Vectors and accounting for the quantum theoretical structure of the periodic table, we created a channel representation of the electron shell structure of atoms. To be able to accommodate four quantum numbers (Table 1), we introduced minor modifications to our notation. A periodic function $f(t)$ can be represented by complex (exponential) form of the Fourier series where:

$$f(t) = \sum_{k=-\infty}^{\infty} c_k e^{ikt} \tag{1}$$

with $\left|c_k e^{ikt}\right| = |c_k|$. The Fourier series of a regular polygon (Robert, 1994) is then given as:

$$f_n(t) = \sum_{k \equiv q(n)} \frac{e^{ikt}}{k^2} \tag{2}$$

By replacing appropriate variables with the quantum numbers in Table 1, we produced our equation 3.

Table. 1. Quantum Numbers and Fourier Matrix Parameters

Parameters	Symbol	Orbital meaning	Range of values
Principal quantum number	n	shell	$n \geq 1$
Azimuthal quantum number (angular momentum) $\ell = 0, 1, 2, 3$ (s, p, d, f)	ℓ	subshell (s orbital is listed as 0, p orbital as 1 etc.)	$0 \leq \ell \leq n-1$
Magnetic quantum number, (projection of angular momentum) $m_\ell = -3, -2, -1, 0, 1, 2, 3$	m_ℓ	energy shift (orientation of the subshell's shape)	$-\ell \leq m_\ell \leq \ell$
Atomic number	A	Number of protons in a nucleus	$1 \leq A \leq 118$
Period Number	y	The row number of the periodic table	$1 \leq y \leq 7$

The following parameters are defined to represent the polygon with the Fourier series: the atomic number A corresponds to the jump step value of the regular polygon, the azimuthal quantum number ℓ corresponds to the number of vertices of the regular polygon, the magnetic quantum number m_ℓ determines the summation interval over which the Fourier series will be calculated, $n \in Z^+$ is the sampling factor for the numerical algorithms, and it determines the number of samples in $t \in [t_0, 2\pi + t_0]$. y is the period number (the row number of the periodic table), and n is the principal quantum number.

Since the resulting Fourier series calculation is the sum of each Fourier term at time t_0, we can now approximate the Fourier series $f_n(t)$ as a specific form of the communication channel U-matrix:

$$u_n''(t) = \sum_{\ell=0}^{n-1} \sum_{m_\ell=-\ell}^{\ell} \frac{2yn^2 e^{i(A+\ell m_\ell)t}}{\left(\frac{A}{n} + \ell m_\ell\right)^2} \tag{3}$$

In this paper, we study only the most simplified scenario of the T-Vectors to generate a U-matrix to represent the valence shells of the periodic table elements, which we could represent mathematically as:

$$u_\ell'(t) = \sum_{m_\ell=-\ell}^{\ell} \frac{2yn^2 e^{i(A+\ell m_\ell)t}}{\left(\frac{A}{n} + \ell m_\ell\right)^2} \tag{4}$$

2.2. Comparison with the Bohr model of the atom

Based on Bohr's model of Hydrogen atom (Bohr, 1913), the radius of the stationary orbits can be calculated with the following equation:

$$r_n = n^2 a_0 \tag{5}$$

The corresponding electron energy levels are expressed by equation (6):

$$E = \frac{-13.6\ (eV)}{n^2} \tag{6}$$

where a_0 =0.0529 nm, which is the Bohr's radius, r_n is electron orbital radius and n is principal quantum number. Based on this model, the electron energy E and orbital radius r_n have two distinctive mathematical

relationships as functions of principle quantum number n. Bohr's model is only successful in describing hydrogen like atoms but has failed to describe other elements. In addition, electron orbitals are known to have n-1 nodes, therefore, for n=3 and higher orbitals, Bohr's radius model is insufficient to describe the actual radial distribution properties of electron orbitals. A better way to describe electron orbital radius is the average of electron orbital radial probability, called expectation value <r>, which is introduced from the current quantum mechanics description of atomic orbital by Schrödinger equation by using wavefunctions (Schrödinger 1926). Specifically, the Schrödinger equation (7) is an eigenvalue equation. The Hamiltonian operator ($\hat{H}$) operates on a function (Ψ, a wave function), and the result equals to a real number (E, energy value) times the same function. The scalar number is called the eigenvalue, and the function is an eigenfunction of that operator. The s orbitals (l=0) can be described using spherical polar coordinates in the form of a radial function $R_{n,l}$ with a radial variable r and a spherical harmonic function Y_{l,m_l} of angular variables θ and ϕ as shown in equation (8) with the assumption they are separable entities:

$$\hat{H}\Psi = E\Psi \tag{7}$$

$$\varphi_{n,l,m_l} = R_{n,l}Y_{l,m_l} \tag{8}$$

The expectation value of the orbit radius ($< r >$) is used to describe the average of radial probability, which resembles the probabilistic expected value of the result (measurement) from an experiment, can be acquired as:

$$< r > = \int \varphi_{n,l,m_l} * \hat{r}\varphi_{n,l,m_l} dV \tag{9}$$

dV in spherical coordinates contains functions:

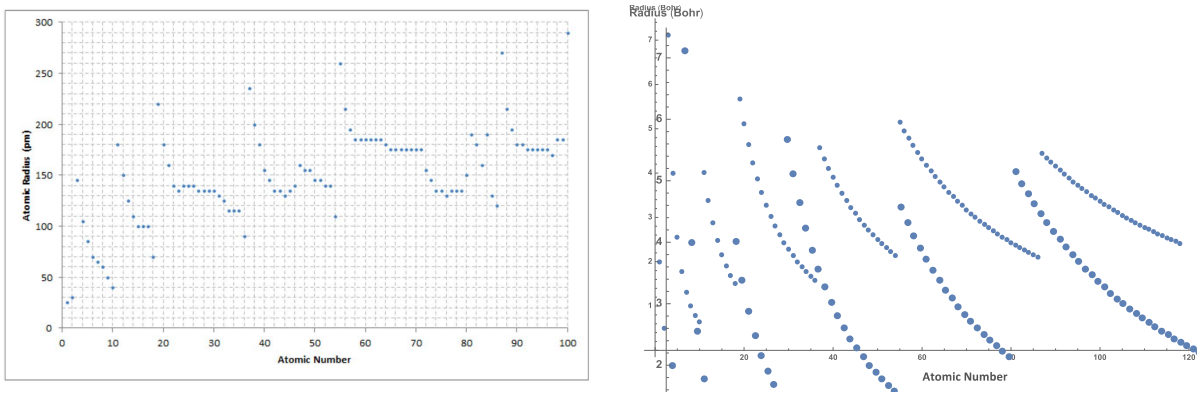
$$dV = r^2 sin\theta dr d\theta d\phi \tag{10}$$

For example, for 1s orbital, the solution from equation (9) gives <r> = $\frac{3a_0}{2Z}$. Heavier atoms are therefore calculated to have a smaller core orbital (1s), and when Z increases the <r> of 1s orbital becomes more compact. Using the U-Matrix Equation (4), we can calculate a general relationship between the orbital radius <r> and the atomic number (Wolfram Curated, 2020, see Figure 5, left). Note, as preliminary work, we focus on the outer valence shell only, and do not attempt to calculate any additional impact of inner shells.

Our results compare favorably with a previous computational study. Bung (Bunge et.al 1993) calculated the <r> values based on Schrödinger equation derived computational model for elements from He up to the fifth period (Figure 5, left). The <r> of s orbitals (1s, 2s, 3s, 4s, 5s) of these elements are also compared with the three dimensional (3D) polygon, polygon jump steps and demonstrate a strong similarity in orbital radius compared to the expectation value <r> defined by Quantum Mechanics (QM) (See Figure 6). Note <r> values are converging from Rb to Xe with the increase of atomic number (Z) and the direction of convergence points towards the jump step derived eigenvalues. The heavier the atom, the more control of nucleus over the electron orbitals and the orbitals are thus more compact. For example, s orbitals (n=1, 2, 3, 4, 5) of Rb are calculated in Wolfram Mathematica (see Table 2).

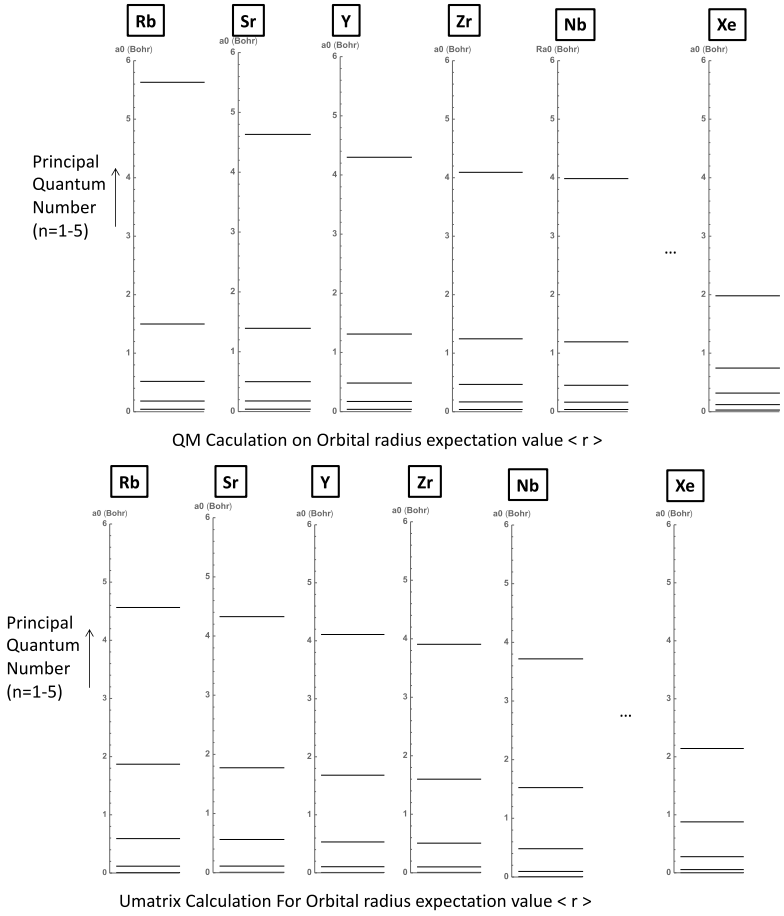
The U-Matrix formulation describes a discrete information content graph for each element; in Figure 7, we again show this information (or error) content graph for the 5th period elements.

The calculated expectation values and error content graphs for all 118 elements in Wolfram Mathematica Notebook are available as an appendix (Link is available SDPS webpage www.sdpsnet.org).



Comparison between empirical value of atomic radius (pm) and U-matrix calculated valence orbitals as the atomic radius for the periodic table of elements. One Bohr= 52.9177pm. Examing the <s> orbital radius only, calculated U-matrix values show a trend parallel to empiric measurements. Adding additional orbitals would be expected to increase graph complexity and estimate precision.

Figure. 5. Empiric Values of Atomic Radius Compared to U-Matrix Calculated Valence Orbital Radius



The U-matrix calculated expectation value <r> (bottom) compares well with QM-derived estimates (top).

Figure. 6. Comparing QM and U-Matrix Calculated s-Orbital Radius Expectation Value <r>

Table 2: Wolfram Mathematical Calculations Generated for Rubidium for Figure 6

```
A = 37;
t = 2 * Pi;
y = 5;
shell = 5;
l = 0
Graphics[{
  Table[{
    Line[{{1, r}, {10, r}}]
   }
   ,
   {r, Table[Max[{Abs[Re[{∑_{m=-l}^{l} 2 * n * n * y * Exp[i (A + m * l) t] / (A / n + m * l)^2}]],
        Abs[Im[{∑_{m=-l}^{l} 2 * n * n * y * Exp[i (A + m * l) t] / (A / n + m * l)^2}]]}], {n, 1, shell, 1}]}]
 },
 Axes → True, Ticks → {None, Automatic}, AxesLabel → {"", "a0 (Bohr)"}
 ,
 PlotRange → {{0, 10}, {0, 6}}
 ,
 AspectRatio → 5

]
```

3. Summary and Conclusion

In this paper, we describe a communication theory inspired scale-invariant model called Communication Dynamics. We demonstrate an application of Communication Dynamics modelling atomic radii for the entire periodic table. In this preliminary study, we developed an initial model using a special form of the Fourier matrix representing communication channels to describe electron shells. We implemented our model in Wolfram Mathematica (Wolfram 2020). We computed the expectation value of the atomic radius using our model. We considered only the outermost shell and ignored interactions with internal shells. Under this assumption, we show favourable agreement with conventional quantum mechanical values and empirical measurements. This model has linear computational complexity and can be scaled to compute other properties of atoms or molecules with a reduction of computational cost with, potentially, higher precision.

Our work seeks to embed an interpretation of the quantum that is consistent with general and special relativity, defined by Einstein. Specifically, the Communication Dynamics approach satisfies the following principles, laid down by Lee Smolin (Smolin 2019).

Principle 1 - Background independence: The Communication Dynamics Theory does not describe substance in the context of a background or any reference system. All consequences arise from consequences of initial axioms and principles utilizing T-Vector.

Principle 2 - Space and Time are Relational: The Communication Dynamics Theory represents spacetime points as complex numbers ($x + it$). The field, now represented by T-Vectors, becomes naturally a spacetime field.

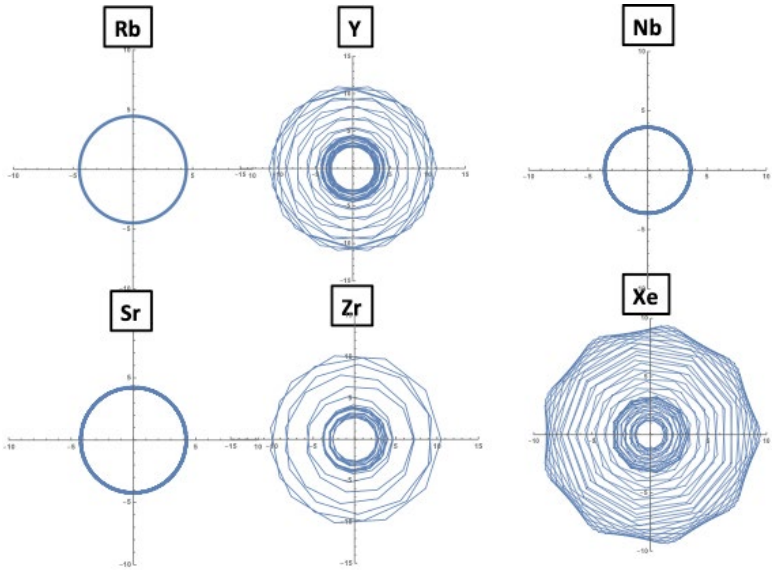
Principle 3 - Causal Completeness: In the Communication Dynamics model, causality is directional and is complete.

Principle 4 - Principle of Reciprocity: In the model, computing processes are reciprocal processes. Any substance is in a dynamic input/output state.

Principle 5 - Identity of Indiscernibles: In the model all objects, even objects that mathematically resemble each other, are unique due to the unique clocks embedded in each T-Vector.

More generally, Communication Dynamics is a model based on first principles, analogous to two prior models based on first principles, the models of Newton (particle interactions) and Maxwell (wave fields). Communication Dynamics describes an information theory-based model of Spacetime using T-Vectors. The model represents a Universe that is frequency based, scale free, and particle agnostic. We claim without demonstration in this paper that particles, such as protons, electrons, and atoms, are emergent observations

that are generated from a fundamental communication system of Spacetime. We demonstrate here an initial practical description of the relevance of our model and will illuminate the model further in future work. We add 141-pages of Wolfram Mathematica computations as an appendix. Another work in this journal, introducing the concept of discrete Planck-scale objects as "observers", makes an initial attempt to generate a hyperbolic visualization of our model and derive, from first principles, fundamental physical constants and forces of nature. Inquiries are welcome.



For example, the communication channel graph of s orbitals (n=1, 2, 3, 4, 5) of Rb are calculated in Wolfram Mathematica as shown below:

```
Rb

DynamicModule[{A = 37, l = 0, n = 5, y = 5}, ListLinePlot[Table[
    {Re[Sum[2 n n y Exp[i (A + m l) t]/(A/n + m l)^2, {m, -l, l}]],
     Im[Sum[2 n n y Exp[i (A + m l) t]/(A/n + m l)^2, {m, -l, l}]]}, {t, 0, 2 π, π/200}],
  Axes → True, PlotRange → {{-10, 10}, {-10, 10}}, AspectRatio → 1]]
```

Figure. 7. Information/Error Content Graphs for 5th Period Elements, as Calculated by the U-Matrix, and Associated Wolfram Mathematica Calculations

4. Dedication and Acknowledgements

This paper is dedicated to three extraordinary people: 1) *Steven Weinberg* for his inspiring words of encouragement in 2010 during the acceptance of his SDPS Medal and attending the Frank Wilczek lecture at UAB; 2) *Frank Wilczek*, the Feynman of our time, for his extraordinary service to the community both inside and outside of the field of physic; and 3) *Stephen Wolfram* for his unrelenting pursuit of computational tools for exploring science and engineering.

We are indebted to Tricia Brown (Georgia Southern University) for her comments and corrections on various versions of this paper. Communication Dynamics Theory evolved over time. More than thirty years ago, Dr. Richard Hamming in 1989 suggested the use of communication theory in systems modeling. Some twenty years ago Dr. Raymond T. Yeh encouraged the development of this theory, and he has continued to be encouraging and supportive. Stan Gatchel generated Society for Design and Process Science logos (www.sdpsnet.org) based

on regular polygons inspired by the special Fourier Matrices of Communication Dynamics. In the intervening twenty years Dr. Murat N. Tanju listened and discussed many aspects of the theory with Murat M. Tanik. Many aspects of this theory developed and applied in the following dissertations, starting in 1978. Saleh Allehaibi, Wireless Communication with Communication Theory, UAB, 2018; Serkan Güldal, Least Action Principle in Information Theory, UAB 2016; Luai Najim, Quantum Computing, UAB 2014; Fan Xiong, A generalized Noisy communication channel Approach for quantum computing, UAB 2013; Bunyamin Ozaydin, An information theoretical modeling and analysis of systems, UAB 2012; Stanley Carl Thompson, Information theoretical Modeling of Complex Systems, UAB, 2008; Ozgur Aktunc, An Entropy Based Measurement Framework for Component-Based Hierarchical Systems; UAB, 2007; Remzi Seker; Component-Based Software Modeling Based on Shannon's Information Channels. UAB 2002; Cengiz Erbas; Modeling and Verification of Real-Time Systems; August, 1994; Chung Pi; N-Queens Problem and Its Relationship to Affine Planes and Error-Correcting Codes; December, 1993; Murat Tanik, A Graph Model for Deadlock Prevention, TAMU, 1978.

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Author Biographies

Lurong Pan (Chief Executive Officer, Ainnocence, Inc) Over the course of a varied academic and business career, Lurong Pan has focused on the application of computational methods to predict biological events, especially for disease pathophysiologies. After graduating with a degree in applied chemistry from Nanjing University, Dr. Pan pursued a PhD in chemistry (specializing in computational chemistry) from the University of Alabama at Birmingham, followed by a post-doc in structural biology while studying for her master's degree in artificial intelligence at Georgia Tech. She helped to build the Integrated System Center of University of Alabama at Birmingham, promoting interdisciplinary biomedical research. She then joined a group of scientists to build the Global Health Drug Discovery Institute, a non-profit founded by

the Bill & Melinda Gates Foundation, Tsinghua University, and the Beijing Municipal government. The team applied AI to discover drugs that could address diseases that affect large populations in the developing world. In 2021, Dr. Pan founded Ainnocence to harness the enormous potential of AI and big data to give scientists a new and accelerated method for conducting drug discovery research — globally and collaboratively — using a highly energy-efficient, accurate, and translational AI drug-discovery platform. Dr. Pan has maintained a longstanding academic collaboration with Dr. Murat Tanik.

Frank M. Skidmore (M.D., Founder, Vice President for Research and Development, Analytical AI, Inc) Dr. Skidmore is a board-certified neurologist who maintains an active neurology practice. As a neurologist, his research has been focused on statistical analysis of brain imaging, focused on using artificial intelligence (AI) as a diagnostic tool for Parkinson's disease, stroke, and other medical conditions. He mentored multiple PhD students, including two who later joined Analytical AI, a company he founded 2018 to develop practical AI applications and where he currently serves as Vice President for Research and Development. Dr. Skidmore developed effective methods for assessing the capability of 3D and higher dimensional imaging data to help diagnose certain neurological conditions, and developed robust statistical methods to understand signal, noise, and statistical power in imaging data. Dr. Skidmore's academic funding included KL-2 and K-23 awards from the National Institutes of Health, innovation awards from the Michael J. Fox Foundation, and computational grants from Oak Ridge National Laboratories. More recent funding has come from the Transportation and Security Agency, Sandia National Laboratories, and the Department of Homeland Security, and the Department of the Airforce. He has published over 70 journal papers, conference papers, review articles, and book chapters and has authored several patents. Dr. Skidmore has maintained a decade-long research collaboration with Dr. Murat Tanik.

Serkan Güldal (PhD, Assist. Prof. in Physics, Adiyaman University) is a full-time faculty in the Physics Department at Adiyaman University. Dr. Güldal received his B.S. in Physics from Erciyes University in 2006. He obtained his master's degree in 2011 Physics from Mississippi State University. In his master's study, he studied molecular mechanics by Density Functional Theory. His PhD is in Interdisciplinary Engineering from the University of Alabama at Birmingham (UAB) in 2016. His PhD research indicates the redefinition of the least action principle outside mechanical physics by information theory. He has been working on research projects on modeling of magnetic materials, machine learning, and synthetic data generation. Also, he has numerous published studies focused on algorithm development. He is a member of the Integrated Systems Center at UAB.

Murat M. Tanik (PhD, Professor of Engineering, University of Alabama at Birmingham) Professor Murat Tanik is the Wallace R. Bunn Chair of Telecommunications at the Department of Electrical and Computer Engineering at the University of Alabama at Birmingham (UAB), and, until recently, served as the Department Chair. In 1978, Dr. Tanik received his Ph.D. degree in Computer Science from Texas A&M University. Before joining UAB in 1998, he had previously taught at Southern Methodist University (SMU), New Jersey Institute of Technology (NJIT), University of Texas at Dallas (UTD) and the University of Texas at Austin (UTAustin). He is co-founder of the Society for Design and Process Science (SDPS), an interdisciplinary society. Dr. Tanik has lectured all over the world as an invited speaker and served as Chief Scientist for two different high technology companies. His industry experience is extensive including Collins Radio, ISSI, and more. He has co-authored six books, co-edited eight collected works, and more than 180 journal papers, conference papers, book chapters, and reports funded by various government agencies and corporations. Under his direction, more than 25 Ph.D. dissertations and 20 M.S. theses have been completed. Beginning in the early 2000's, Dr. Tanik increasingly devoted his research time to the development of a communication-theory based approach to computing which led Communication Dynamics Theory.