**Technical Proposal**

**Specific Aims**

Defining optimality and ensuring global optimal performance for a complex system of systems is a challenging, active area of research. These challenges are exacerbated when humans are components in such systems: while humans excel at learning and are adept at generalizing experiences to solve new problems, human behavior is often irrational and human processing speeds are comparatively slow and unpredictable at performing certain tasks (e.g., due to cognitive depletion).

This work has three main objectives:

1. Develop and demonstrate the mathematical foundations to identify the optimal roles and actions for all components in a complex system of systems where components actions are well defined.
2. Extend this work to define optimality in a streaming system of systems. In comparison components considered in the previous task, components in these systems must make decisions based on incomplete information (i.e., information based on sampled data streams). We thus extend optimality to account for irrationality based on lossy information.
3. Finally, extend these foundations to define optimality for dynamic systems that transition between states. In such systems, the roles of components may change based on the state the system is operating in.

We anticipate no less than 2 publications on these results, and will be working to assist the EM use-case.

**Background and Significance**

Decision theory is the mathematical framework to determine the best course of action to take from an array of possible actions. A critical element to this research is that the consequences (or rewards) for any choice are uncertain. Formally, a decision problem involves a set, , of states or outcomes of the decision (e.g., success and failure of a coin flip, or the outcomes of a die roll: 1,2, ... ,6) and a set, ,of consequences. The decision, , maps each element in the state space to an outcome (e.g., a consequence or a payoff): . Based on the states and outcomes, the decision maker must decide to proceed with the choice or not. For example, in its simplest form there is some probability distribution *p* on such that the expected utility of a given decision is expressed:

Equation

Where is the utility function that maps each potential consequence of the decision,, to a real value (e.g., dollars earned or lost, crops gained, etc.): . Thus the expected utility of a decision is the sum of all possible rewards and penalties for each outcome multiplied by the probability of the outcome occurring. Note that there may be several decisions to choose between, , each with its own set of outcomes, , with corresponding probability distributions , consequences, ,and utility functions, . In this context, the decision maker must assess the expected utility of each decision , where is the set of all possible decisions, to choose the most optimal .

From early works in the 17th century (Bernoulli 1954), decision theory has matured and is actively researched today, consisting of many specialty areas: *selection uncertainty*, which represents the core of decision theory; *intertemporal choice theory*, which is concerned with decisions where outcomes and utility of a choice is realized at different points of time; *interaction theory,* which examines decisions that are effected by the response of other agents/individuals in the situation; and, complexity theory, which addresses decisions that are difficult simply because of their complexity, or the complexity of the organization that has to make them. In all of the above examples, the focus of the theoretical challenge is the study of how an agent can maximize its expected utility in situations where there are no other agents making choices. Even in interaction theory, the problems are typically phrased from the point of a single individual and how response actions of others to their choice play into a decision.

Game theory expands on decision theory to address how multiple competing agents should engage so that all players reach their maximum expected utility. Formally, in noncooperative games, each agent’s set of decisions, state set, and consequence set, must account for the actions of the other agents. The challenge is to determine the set of decisions for all competing agents that maximize each agent’s expected utility (Equation 1). In these systems, player is rationality is defined as a player that is aware of all states, consequences, and utility of the other players. Given this knowledge, the player will *rationally* choose the decision that is their most optimal. If all players in a noncooperative game are rational, Nash equilibrium (Osborne and Rubinstein 1994) guarantees the existence of an optimal solution such that each player is guaranteed with the best possible outcome.

With such guarantees for optimality, the internal consistency and mathematical foundations of game theory make it uniquely capable to model and design automated decision-making processes in interactive environments. For example, to design an efficient set of bidding rules for an auction website, or tamper-proof automated negotiations for purchasing communication bandwidth.

Despite the broad applicability of game theory, research in applied game theory is still a nascent component in contemporary conference and journal papers (Lorentziadis 2016). One of the more significant challenges faced by these applications is the notion that for many systems, assumptions of bounded rationality do not realistically capture the behavior of real world systems. For example, there are few cases where an agent is fully aware of the states, decisions, and consequences of their opponents. Decisions made by a player under these cases may be intended to be rationally, but as they are based on partial or incorrect beliefs of the player’s opponents, the decisions will ultimately be irrational.

This project will address the challenges of how to help refine a player’s beliefs about their opponent’s decision, state, and consequence sets. By providing a framework to refine incorrect or partial beliefs in a streaming environment, BIFROST will help to refine the inherent irrationality seen in many games and players towards a more rational system where a known optimal solution for players is known to exist.

**Research Design and Methodology**

The research for this project supports two fundamental objectives: the development of a mathematical foundation that can map irrational systems to rational systems; and, the application of this methodology to a streaming system to demonstrate the methodology’s benefits. We now discuss our research approach for developing the methodology.

Objective 1: Develop a Mathematical Foundation to Bridge Between Irrational and Rational Games

Under bounded rationality in a noncooperative game, player is able to accurately assess their respective expected utility for each possible decision in their set of possible decisions, . Accuracy in this decision-ranking task is based on the fact that this player understands the decision sets and corresponding expected utility of each opponent. However, the expected utility of each decision may be falsely derived if any of the following properties do not hold:

* The decision set of all players is known
* Each decision’s states and consequences, are known
* Each decision’s probability distribution, on is known
* Each decision’s utility function, is known

The BIFROST framework will address three common violations for bounded rationality that prevent a system from reaching an optimal equilibrium. Working with simple 2 and 3 player games, we build our framework to address the following violations.

1. **Case 1:** The decision set of one or more players is unknown. For example, player 1 and 2 may be operating in a fully rational manner, but player 3 may have a strategy that is unknown to players 1 and 2.
2. **Case 2:** The probability distribution on is unknown. For example, in a two player game of dice, player two may have loaded dice such that the probability of states occurring is not 1/6.
3. **Case 3:** The states and consequences, of a given decision are incomplete.

To address these challenges, we propose a learning-based approach to support transitioning irrational systems (i.e., systems where players are not rational) to more rational systems. Formally, the hypothesis of this work is that a player can *learn* when their expected utility is not optimal by detecting specific features that are associated with the above cases. For example, detect when an opponent’s distribution on dice rolls is not uniformly distributed. In this manner, when detecting a potential violation of bounded rationality, the player can attempt to learn the more correct behavior; e.g., change their assumed distribution of dice rolls from uniform to the observed distribution. In this context, BIFROST will serve to *rationalize* systems that are irrational to ensure that an optimal state for all agents may be reached.

We address these specific cases based on the following proposed tasks.

**Task 1: Background Research -** Undertake a literature search to identify how game-theory and learning methodologies can be fused to help address the challenges associated with implementing a learning-based approach for game-theory.

**Outcome of Task 1 -** If the findings are substantial enough, the outcome will be a literature review paper, otherwise, a technical report that will provide background and introductory material for other papers.

**Task 2: Define Mathematical Formalism for BIFROST –** Define the formalism that will integrate existing aspects of decision theory, information theory, uncertainty characterization, machine learning, and game theory to support a learning-based game theoretic approach. Subtasks for this work will be based on the cases discussed above:

**Task 2.a** Extend BIFROST to help agents detect and adapt to unknown decisions being made by opponents

**Task 2.b** Extend BIFROST to help agents detect and adapt to unknown states and consequences, of an opponent’s decision.

**Task 2.c** Extend BIFROST to help agents detect and adapt to incorrect assumptions about an opponent’s probability distributions on **.**

**Outcome of Task 2 -** A technical report and corresponding journal article that describes how to implement the learning-based optimization for game theoretic models. This technical foundation will be the cornerstone of this project’s work and represents a novel contribution for AIM research. Additionally, each subtask will represent a new code update to the BIFROST repository; this update will include the new capability as well as a suit of simulations and data to demonstrate the specific capability.

**Task 3: Lexicon –** Define the complete set of terminology necessary to discuss game theory within the context of the AIM Lexicon.

**Outcome of Task 3 -** A document containing the lexicon for game theory that will provide a working vocabulary for this project and will seamlessly integrate and extend the terminology used by AIM.

Objective 2: Demonstrate Benefits of Methodology for Hierarchical Signature Detection

The second objective of this project is to demonstrate the benefits of the methodology developed in Objective 1 by applying it to the decision processes behind the JEOL electron microscope (EM).

**Task 4: Become Familiar with EM use case –** Work with CoPIs to completely landscape the and needs of the computational capabilities of the JEOL EM. Identify the limitations and best approaches from Task 2 that will likely be needed to address the various detection tasks.

**Outcome of Task 4 -** A practical understanding of how the JEOL EM works and how to deploy the BIFROST framework onto this device.

**Task 5: Validate BIFROST on JEOL EM data –** Based on Task 4, demonstrate BIFROST on captured JEOL experimental data.

**Outcome of Task 5 –** Demonstrated BIFROST framework on JEOL offline data.

**Task 6: Deploy Hierarchical Signature for Particle Detection –** Based Task 5, deploy BIFROST to the JEOL EM to help guide steering.

**Outcome of Task 6 –** Demonstrated BIFROST on streaming system.

**Task 7: Analysis Presentation of Results –** Based on outcomes for Tasks 1-5 journal publications will be submitted.

**Technical Milestones**

**FY16**

**End of Q2**

Complete Task 1: Background Research

Task 2.a: Complete first stage of BIFROST code to adapt to unknown decisions

Task 3: First pass of lexicon completed

Task 4: Develop strategy for BIFROST integration into JEOL EM

**End of Q3**

Complete Task 2b: Complete first stage of BIFROST code to adapt to unknown states and consequences

Task 2c: Complete first stage of BIFROST code to adapt to unknown probability distributions

Task 3: Updates to lexicon

Task 5: Demonstrate BIFROST on offline JEOL EM data

**End of Q4**

Complete Task 6: Demonstrate BIFROST on JEOL EM

Task 3: Final update to lexicon

Task 7: Papers published (survey and technical)

**FY17: Contingent to FY17 funding, BIFROST will be applied to a 2nd application space (application TBD)**

**Key Staff**

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| **Name** | **Role** | **Expertise / Domain Area** |
| Luke Gosink | Principal Investigator | Computer Science |
| Jenny Webster | CoPI | Math |
| Kathleen Nowak | CoPI | Math |
| Sam Chatterjee | CoPI | Civil Engineering / Operations Research |

We do not expect that we will make use of subcontracts or partnerships outside the lab at the time of the proposal.

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| **BIOGRAPHICAL SKETCH** | | | |
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| **Education/Training** | | | |
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| University of California, Davis | B.S. | 1996 | Chemistry |
| University of California, Davis | Ph.D. | 2009 | Computer Science |

*Appointments*

* *Pacific Northwest National Laboratory, Research Scientist, Statistics and Sensor Analytics, 2010-present*
* *Lawrence Berkeley National Laboratory, Graduate Research Associate, Scientific Visualization Group, 2004-2010*
* *ZWorld / Rabbit Semiconductor, Software Quality Assurance manager, 2000-2004*
* *Axys Pharmaceuticals, Research Associate, 1996-2000*

*Publications*

* *L. J. Gosink, J. C. Anderson, C. Garth, E. W. Bethel, and K. I. Joy, “Multivariate Distribution-Based Segmentation for Query-Driven Visualization”, IEEE Trans. on Visualization and Computer Graphics, 2011.*
* *L. J. Gosink, K. Wu, E. W. Bethel, J. D. Owens, and K. I. Joy, “Data Parallel Bin-Based Indexing for Answering Queries on Multi-Core Architectures”, International Conference on Scientific and Statistical Database Management, 2009.*
* *J. C. Anderson, L. J. Gosink, M.A. Duchaineau, and K. I. Joy, “Interactive Visualization of Function Fields by Range-Space Segmentation”, in Proc. of EuroVis, 2009.*
* *L. J. Gosink, J. C. Anderson, E. W. Bethel, and K. I. Joy, “Query-Driven Visualization of Time-Varying Adaptive Mesh Refinement Data”, IEEE Trans. on Visualization and Computer Graphics, 2008.*
* *L. J. Gosink, J. C. Anderson, E.W. Bethel, and K. I. Joy, “Variable Interactions in Query-Driven Visualization”, IEEE Trans. on Visualization and Computer Graphics, 2007. — Nominated for a best paper award at the IEEE Vis Conference*

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| University of California, San Diego | B.A. | 2008 | Applied Mathematics (Honors) & History |
| Texas A&M University | Ph.D. | 2013 | Applied Mathematics |

*Appointments*

* *Pacific Northwest National Laboratory, Research Scientist, Applied Statistics and Computational Modeling, 2013-present*
* *Texas A&M University, Graduate Student Research Assistant (DHS DNDO grant), 2008-2012*
* *Blinn College, Learning Center Tutor, 2011*
* *Los Alamos National Laboratory, Student Intern (undergraduate and graduate), Applied Physics Division and Computational & Statistical Sciences Division, 2004-2011*

*Publications*

* L. E. Smith, K. A. Miller, J. R. Garner, S. Branney, B. S. McDonald, J. B. Webster, M. A. Zalavadia, L. C. Todd, J. A. Kulisek, H. Nordquist, N. S. Deshmukh, and S. Stewart, Viability study for an unattended uf6 cylinder verification station: Phase I final report, Tech. Report PNNL-25395, Pacific Northwest National Laboratory, 2016.
* P. S. Mackey and J. B. Webster, A multi-network analysis of scientists on social media and their scientific co-authorship graphs, in SIAM Workshop on Network Science (NS16), Boston, MA, 2016.
* J. B. Webster, Fundamental mathematical models for human interactions, Tech. Report PNNL-SA-118712, Pacific Northwest National Laboratory, 2016.
* J. B. Webster, Understanding data: Graphs and their uses, in SIAM Annual Meeting, Boston, MA, 2016.
* A. M. B. Peddicord, D. W. Engel, Z. N. Gastelum, A. Heredia-Langner, E. A. Hogan, V. A. Lewis, K. E. McNeil, L. R. Rodriguez, and J. B. Webster, Signature discovery for procurement networks in business intelligence applications, Tech. Report PNNL-24554, Pacific Northwest National Laboratory, 2015.
* J. B. Webster, Cost-sensitive classification methods for the detection of smuggled nuclear material in cargo containers, in Information Analysis Technologies, Techniques, and Methods for Safeguards, Nonproliferation and Arms Control Verification Workshop, INMM, May 2014, pp. 184–199.
* M. Allmaras, W. Bangerth, J. M. Linhart, J. Polanco, F. Wang, K. Wang, J. Webster, and S. Zedler, Estimating parameters in physical models through bayesian inversion: A complete example, SIAM Review, 55 (2013).

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| University of New York, Geneseo | B.A. | 2010 | Mathematics |
| Iowa State University | Ph.D. | 2015 | Mathematics |

*Appointments*

* *Pacific Northwest National Laboratory, Research Scientist, Computational Mathematics, 2015-present*

*Publications*

* *Paul Bruillard, Kathleen Nowak, Emilie Purvine, “Anomaly detection using persistent homology”, To appear in Annual Cybersecurity Symposium Conference Proceedings.*
* *Kathleen Nowak, Oktay Olmez, Sung Y. Song, “A family of partial geometric designs from three-class association schemes”, To appear in Journal of Combinatorial Designs.*
* *Keivan Hassani, Paul Horn, Franklin Kenter, Kathleen Nowak, John Sinkovic, Josh Tobin, “On the principal permanent rank characteristic sequences of graphs and digraphs”, Electronic Journal of Linear Algebra 31 (2016), 187–199.*
* *Kathleen Nowak, Oktay Olmez, “Partial geometric designs with prescribed automorphisms”, Designs, Codes, and Cryptography 80 (2016), no.3, 435–451.*
* *Kathleen Nowak, Oktay Olmez, Sung Y. Song, “Partial geometric difference families”, Journal of Combinatorial Designs, 24 (2016), no. 3, 112–131.*
* *Chassidy Bozeman, AnnaVictoria Ellsworth, Leslie Hogben, Chin-Hung Jephian, Gabi Maurer, Kathleen Nowak, Aaron Rodriguez, James Strickland, “Minimum rank of graphs with loops”, Electronic Journal of Linear Algebra 27 (2014) 907–934.*

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| **BIOGRAPHICAL SKETCH** | | | |
| **Name** (Last, first, middle initial)  Chatterjee, Samrat | | **Position Title**  Scientist | |
| **Education/Training** | | | |
| **Institution and Location** | **Degree** | **Year(s)** | **Field of Study** |
| Punjab Engineering College, India | B.E. (Honors) | 2003 | Civil Engineering |
| University of Texas, Austin, TX | M.S.E. | 2006 | Civil Engineering – Infrastructure Systems |
| Vanderbilt University, Nashville, TN | Ph.D. | 2010 | Civil Engineering – Infrastructure Systems; Risk and Decision Analysis |
| University of Southern California, Los Angeles, CA | Postdoc | 2010-2014 | Homeland Security Risk and Decision Analysis; Operations Research/Statistical Modeling |

*Appointments*

* *Pacific Northwest National Laboratory, Operations Research Scientist, 2014-present*
* *University of Southern California, Postdoctoral Research Associate, CREATE Homeland Security Center of Excellence, 2010-2014*
* *Vanderbilt University, Graduate Research Assistant, Department of Civil and Environmental Engineering, 2006-2010*

*Publications*

* *Chatterjee, S., M. Halappanavar, R. Tipireddy, and M. Oster. (2016) Game theory and uncertainty quantification for cyber defense applications. SIAM News, 49(6).*
* *Chatterjee, S., R. Tipireddy, M.R. Oster, and M. Halappanavar. (2015) A probabilistic framework for quantifying mixed uncertainties in cyber attacker payoffs. National Cybersecurity Institute Journal, 2(3), 13-24.*
* *Bramer, L.M., S. Chatterjee, A.E. Holmes, S.F. Bradley, S.M. Robinson, and BJ. M. Webb-Robertson. (2015) A machine learning approach for business intelligence analysis using commercial shipping transaction data. In Proceedings of the International Conference on Data Mining, Las Vegas, NV, 162-167.*
* *Chatterjee, S., S.C. Hora, and H. Rosoff. (2015) Portfolio analysis of layered security measures. Risk Analysis, 35(3), 459-475.*
* *Chatterjee, S., M. Halappanavar, R. Tipireddy, M.R. Oster, and S. Saha. (2015) Quantifying mixed uncertainties in cyber attacker payoffs. In Proceedings of the IEEE International Conference on Technologies for Homeland Security, Waltham, MA, 1-6. Best Paper Award (Cyber Security).*

**General Business Strategy**

Department of Homeland Security (DHS)

National Nuclear Security Administration (NNSA)

Department of Defense (DoD)

Office of Counter Intelligence (DOECN)

Office of Intelligence (DOEIN)

Numerous organizations, both in the public and private sectors, require the ability to support efficient decision making that must rank multiple, complex and often competing demands for resources and capabilities. This project’s principal business strategy is to clearly demonstrate the efficacy and impact of BIFROST to support real-time optimal decision support for resource use, capability development and deployment. Success in these areas will make PNNL more competitive for follow-on funding to a wide array of clients who are attempting to construct and deploy their own control processes. Solid publications will be an essential part of establishing PNNL’s leadership and expertise in this area. Lessons learned in the LDRD project lifespan will allow us to develop and refine general techniques that can then be applied outside the initial application spaces. We intend to communicate regularly with sector managers and keep them informed of our progress. Additionally, where appropriate, we will approach and interact with clients during the course of the project to solicit external interest and support.

Go to the [LDRD Tool Suite](https://ldrd.pnl.gov/ToolSuite/Default.aspx), select “Start a Data Sheet”, enter the required information, and upload your proposal. **All LDRD projects must maintain a “data sheet” containing specific information per DOE Order 413.2B. The purpose of the data sheet is to provide information to DOE and Congress and is used for federal sign-off on all LDRD projects. The information below is part of the data sheet and will be shared outside of PNNL. This should not include any proprietary information.** The other information in the data sheet form is self-explanatory. You will also need to complete these fields:

**Abstract**

Formally defining optimal performance for a streaming complex system of systems is challenging. Operational components in these systems include a diverse array of roles including: human decision makers and analysts tasked with maintaining situation awareness, machine learning methods that are critical for timely analysis tasks, and sensors that sample the environment based on different sensing and sampling modalities. These components must complete their individual tasks under the constraints of shared, limited resources: e.g., compute resources, bandwidth, cache, etc. Optimal global performance therefore requires identifying the best approach for sharing resources to complete a global task.

This project will model the analysis processes and potential actions preformed by such complex streaming systems as an Informational Theoretic (IT) problem (Wolpert 2006). In this framework, each process is treated as a player in a non-cooperative game. Bounded rational game theory asserts that each of these players is fully “rational” and aware of the possible actions of every other player as well as the penalties and rewards of these actions. Based on each players assured rationality, this theory ensures the existence of an optimal, stable state for the system as a whole (i.e., the Nash equilibrium (Osborne and Rubinstein 1994)); any alternate state is guaranteed to result in degraded performance of the system. Importantly, this theory identifies the actions required of each process – both human decision makers and machines.

If this work is successful in casting the streaming analysis problem in an IT framework, we will be able to analyze any system and provably define the best course of action for each component in the system. More specifically, we will be able to identify how humans and machines will be able to best work together for the learning of complex processes and the analysis of streaming data streams.

**Summary of Expected Outcomes**

The outcomes of this project will be: 1) a mathematical framework and code base to support detecting irrational systems and refining the underlying knowledge of these systems to transition them to bounded rational systems, and 2) the demonstrated benefits of this methodology through its application to the JEOL EM use case. These outcomes will be realized through the completion of several intermediate outcomes. We identify both primary and intermediate outcomes below.

* General methodology
  + Develop a formalism consisting of mathematical and natural language descriptions that define the way optimality, control, and learning frameworks are discussed, designed, and implemented.
    - Additions to the AIM Lexicon
    - Documentation defining formalism
  + Identify and develop methods for quantifying propagated error and uncertainty for irrational systems.
    - Publications targeting error and uncertainty for irrational systems
  + Provide software code and algorithms that can interface with a broader computational framework, to assist in implementing BIFROST generally for any system.
* Demonstration of Methodology
  + Develop an instance of BIFROST to run on the JEOL EM. By optimizing the way that humans, analytics, visualization, and data from JEOL experiments interact, BIFROST will help to reduce the time subject matter experts must spend in calibrating the EM and running experiments.
  + Publications documenting the applied method.