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Accomplishments

* What are the major goals of the project?

The rapidly growing complex network science has presented novel approaches to complex systems modeling that were not fully foreseen even in a few decades ago. It addresses the self-organization of complex network structure and its implications for system behavior, which holds significant cross-disciplinary relevance to many fields of natural and social sciences, particularly in today’s highly networked social/political/economical circumstances.

Interestingly, complex network science has traditionally addressed either "dynamics on networks" (state transition on a network with a fixed topology) or "dynamics of networks" (topological transformation of a network with no dynamic state changes) almost separately. In many real-world complex biological and social networks, however, these two dynamics interact with each other and often coevolve over the same time scales. Modeling and predicting state-topology coevolution is now recognized as one of the most significant challenges in complex network science.

The goals of this NSF-funded project were to establish a generalized modeling framework that could effectively describe state-topology
coevolution of complex adaptive networks and to develop computational methods for automatic discovery of dynamical rules that best capture both state transition and topological transformation in empirical data. To achieve these goals, graph rewriting systems were used as a means of unified representation of state transition and topological transformation. Network evolution was formulated in two parts, extraction and replacement of subnetworks. For each part, algorithms for automatic rule discovery were explored and developed. Their effectiveness was evaluated through application to simulated and real-world network data.

* What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?

Major Activities:

This project has produced a novel theoretical framework and a computational toolkit that are expected to become the basis of transformational ways of studying the coevolution of dynamics on and of complex networks in the coming years. The developed framework has served as a generalized conceptual/mathematical "language" for modeling, analyzing and discussing the dynamics of various complex systems, which has galvanized interdisciplinary discussion and collaboration across many different areas of applications.

As a computational toolkit, we designed and developed PyGNA, a Generative Network Automata (GNA)-based modeling and analysis framework using Python and the NetworkX module. The development is being done using github.com, a widely used open-source software development website, where all source codes are publicly available for free (https://github.com/schmidtj/PyGNA).

In the final year (2013-2014), we have made a major improvement to PyGNA. Using the work done thus-far as a foundation, we adapted the method to work with real world temporal network data. The majority of this work was done to address scalability issues when transitioning to larger real world data sets. To address the computational complexity of the subgraph isomorphism problem, we have implemented a G-Trie for enumerating subgraphs (https://github.com/schmidtj/G-Trie). The G-Trie also provides us the capability of sampling isomorphic subgraphs, further increasing our ability to analyze larger temporal network data.

See the "Products" section to see more details of the most recent version (ver. 0.8) of PyGNA.

[Testing algorithms with temporal network data]

We conducted experiments applying PyGNA to two different types of data: (1) data generated by abstract adaptive network models, to test if it could correctly identify the actual network generation mechanisms used to produce the input data, and (2) larger-scale real-world temporal network data, to test the scalability of PyGNA and identify technical challenges in scaling up the algorithms. The latter one is a new research activity during the final year (2013-2014).

For the first type of data, the following four abstract adaptive network models were used as inputs to PyGNA:
(a) Barabasi-Albert network, grown using the standard degree-based preferential attachment method.
(b) "Degree-state" network, grown by degree-based preferential attachment applied only to the subset of nodes that have a particular state. Each newly added node is assigned a randomly selected state.
(c) "State-based" network, grown by random attachment only to nodes that have a particular state. Again, each newly added node is assigned with a randomly selected state.
(d) "Forest fire" network, generated by the method proposed in the literature.

For the second type of data, we obtained the temporal network data set of venture capital investors from Dr. Dimo Dimov at the University of Bath, UK. This data set includes 35,757 first-round investments made by 2,498 US-based VC firms between 1980 and 2004, making a total of 24 network snapshots (one for each year). This testing was conducted during the final year of the project (2013-2014).

For each type of data sets, we applied PyGNA to construct adaptive network models and then use them to simulate the network evolution. We then quantified the accuracy of the reconstructed network evolution by using several measurements, including the numbers of nodes and edges, the resulting degree distributions and the frequency distributions of extracted subgraphs. For the latter, we counted how many times each of the different kinds of subgraphs was selected for graph rewriting events in the original input data and the reconstructed network simulation results. The Bhattacharyya distance was then computed between the two distributions.

In the initial testing experiments, both input and reconstructed networks had visually similar structures for the Barabasi-Albert (a), degree-state (b) and state-based (c) networks. For the forest fire network (d), however, PyGNA failed to capture the unique topological characteristics of the original input network, because of the complexity in the original network generation method. The accuracy of the reconstructed network models was also characterized by measuring the Bhattacharyya distance (BD) of frequency distributions of extracted subgraphs between original and reconstructed networks. The BD was low for (a) and (c), while it was high for (b) and (d). We learned from these results that the initial algorithm in PyGNA was effective for certain types of networks while still limited for the analysis of others, especially those that involve pure randomness and/or mesoscopic topological structures such as motifs.

To address these problems, we implemented major improvements in the algorithms of PyGNA. One substantial extension made to the extraction mechanism detection algorithm (which was realized through intensive discussions with Dr. Gross during our stay at the University of Bristol) was to use a motif-based likelihood calculation, instead of a node-based one that was originally adopted. This improvement led to a significant increase in the performance of PyGNA's automated model building abilities. The reconstructed networks looked much closer to the original input networks than before, and both the extracted subgraph distributions and the cumulative degree distributions matched
In applying the motif-based PyGNA to the analysis of the VC investors network data, we encountered several challenges. First, the number of subgraph rewriting events between two consecutive time points was typically very large, and many of them were intractably large subgraphs because of topological overlaps among microscopic rewritings. Second, finding every instance of a particular motif within a large network was computationally not feasible if we used straightforward algorithms.

In the final year of the project (2013-2014), we grappled with these challenges, and made some algorithmic breakthroughs. Since it was practically impossible to record the whole subgraph rewritings in full detail, we adopted a motif sampling approach with bounded motif size instead. Moreover, to achieve drastic improvement in the speed and efficiency in motif search, we developed a Python implementation of the G-Trie motif enumeration algorithm proposed by Ribeiro and Silva (2010). These algorithmic improvements have made it possible to run PyGNA's automated model building process to a large-scale temporal network data set in a practical computational time.

The results showed a reasonably good match between the real-world input data and the simulated data generated using the automatically acquired adaptive network model in some network metrics. In the meantime, we also identified limitations in the current algorithm design that prevented more accurate model building. One fundamental limitation is that our current simulation algorithm excludes possibilities of overlapping rewriting events, even though the motif sampling method we used did capture dynamics made of overlapping rewriting events. This mismatch caused a deviation of the distributions of simulated events from those of actual rewriting events. We will continue working on further algorithmic improvements to address this limitation so that PyGNA can capture the temporal network dynamics more faithfully.

Specific Objectives:  [Collecting real-world network data]

Real-world network evolution data are necessary for evaluating our algorithms. We developed an original web search engine based method for collecting approximated historical data of temporally changing social adaptive networks. In our method, a search query string is combined with additional keywords that specify the inclusion/exclusion of specific years to limit the search results to a particular time point. Using the proposed method, we reconstructed the temporal evolution of a social network from 2005 to 2009 of 93 individuals who are important in the US economy as a test case.

We also used this method to reconstruct a network that represents the relatedness between scientists and their peers as well as various research topics. We characterized each individual scientist's most notable research topics (expertise) by measuring a "visibility boost", defined as the increase of the scientist's visibility resulting from focusing on a particular research topic. We analyzed the correlation between scientists' expertise and their interdisciplinary nature. The interdisciplinarity of a
scientist was characterized in two different ways: (a) diversity in their expertise (i.e., how many research topics they are associated with), and (b) their betweenness centrality in the scientists’ network (i.e., how much they connect multiple scientific communities). While this research did not consider the dynamical nature of the network, it did demonstrate the effectiveness of our data collection method.

Furthermore, we have been working with our collaborators to collect other types of real-world adaptive network data (Dr. Zhirong Bao at Memorial Sloan-Kettering Cancer Center for the data of spatial cellular network evolution over the embryogenesis of C. elegans, and Dr. Dimo Dimov at the University of Bath, UK, for the data of VC investors, as described above). The second data set was much larger than other data sets, and thus we used it for the testing of PyGNA.

[Expanding domains of application]

(a) Adaptive network models of social network evolution. We developed an agent-based model of idea-exchanging social networks to investigate the relationship between individual behavior of agents and their contribution to collective idea generation. Our individual agents divide their time into three distinct actions: thinking about and reconciling one’s own ideas, disseminating ideas to others, and listening to ideas from one’s peers. Each individual is host to a local population of ideas, some of which are fixed, while others can be replaced as a result of social interaction. Individuals evaluate ideas based on their local idea population, and these evaluations are used to update the (directed) link weights whenever ideas are exchanged.

We implemented a parallel simulation platform based on a server-client architecture for this experiment. Using this model and its simulation platform, we conducted exhaustive parameter sweep experiments, calculating the distribution of network centrality of agents and other measurements of their idea contribution.

(b) Adaptive network models of corporate merger. In collaboration with Dr. Junichi Yamanoi at Chuo University, Japan, we developed an adaptive network model of cultural integration in merging firms, represented as a network initially made of two communities. Nodes receive information from their neighbors and update their cultural states, while the link weights also change so that links between nodes with similar/different cultural states are encouraged/discouraged. We investigated the impact of network structures within and between two merging firms on post-merger cultural integration and organizational dysfunctions—individual turnover, interpersonal conflict and organizational communication ineffectiveness—that arise from insufficient cultural integration.

(c) Adaptive network based models of collective behavior of swarms. In collaboration with Dr. Thilo Gross, we developed an adaptive network-based analytical model that represents interaction networks of marching locust swarms that may switch the direction of motion between left and right. Dr. Gross’s recent work considered phase transitions in a homogeneous swarm. We extended their model to heterogeneous swarms made of multiple types. To facilitate analytical work, we developed a computer program that automatically generates all the network rewriting rules from a smaller set of model assumptions, and also a set of dynamical equations that describe dynamical change of network motif densities using a technique called moment
(d) Incorporation of GNA into network models of joint technological systems. We established a research contract with Defence Research and Development Canada Centre for Operational Research and Analysis (DRDC-CORA) to develop GNA-based computer simulation models and analysis tools of the behavior of dynamical operational networks made of heterogeneous specialized agents, each working in distinct environmental domains. A target problem is the SAR (Search and Rescue) operational network for the Canadian Arctic. This project was the first instance of real-world applications of our GNA framework used in non-academic domains. In collaboration with Dr. Irene Pestov at DRDC-CORA, we developed OpNetSim, an adaptive network-based computer simulation model of the behavior of dynamical operational networks. The final simulator software and its user's manual were produced and delivered to DRDC-CORA as specified in our contract.

(e) Adaptive network models of global state drift in social diffusion. We developed adaptive-network models of social diffusion where node degrees are artificially correlated with node states through adaptive link adjustment. In these models, node states diffuse through links in the form of non-conserved social diffusion (i.e., a node's state tends to approach the average of its neighbors' states). In addition, network topology was adjusted based on node states. Two different models were tested. The first model is a discrete-time one, where a small number of links are randomly chosen and removed from the network in each iteration and replaced by the same number of new links between nodes that are selected preferentially based on their states. The second model is a continuous-time one, where link weights gradually increase or decrease based on the node states. We applied these mathematical models to study the effects of such adaptive rewriting on the global drift of average states, especially in the context of education, where nodes, states and links represent students, their grades and their friendships. The second model (continuous-time model written in differential equations) was developed in the final year (2013-2014), whose dynamics were analyzed mathematically as well as using numerical simulations.

(f) Adaptive network approach toward distributed self-control of networked dynamical systems. We have developed mathematical models of distributed control mechanisms for a coupled linear dynamical system, with which the system itself can adjust link weights dynamically using local information only so that it will converge to a desired state spontaneously. We have developed and tested a new second-order control mechanism that uses the difference between the current "direction" of state movement and the desired "direction".

Significant Results: [Testing algorithms with temporal network data]

(See "Major Activities" section)

[Collecting real-world network data]

Using our web search engine-based data collection method, we reconstructed the temporal evolution of a social network from 2005 to 2009 of 93 individuals who are important in the US economy. We measured centralities of those individuals for every year and found several illustrative cases where
the temporal change of centrality of an individual correctly captured the actual events that are related to him/her over this time period. These results indicate the effectiveness of the proposed data collection method.

We also used our data collection method to reconstruct a network that represents the relatedness between scientists and their peers as well as various research topics. We found that researchers who had high "visibility boosts" by the same research topic tended to be close to each other in their network. We calculated correlations between visibility boosts by research topics and researchers' interdisciplinarity at the individual level (diversity of topics related to the researcher) and at the social level (his/her centrality in the researchers' network). We found that visibility boosts by certain research topics were positively correlated with researchers' individual-level interdisciplinarity despite their negative correlations with the general popularity of researchers. It was also found that visibility boosts by network-related topics had positive correlations with researchers' social-level interdisciplinarity. Research topics' correlations with researchers' individual- and social-level interdisciplinarities were found to be nearly independent from each other. These findings suggest that the notion of "interdisciplinarity" of a researcher should be understood as a multi-dimensional concept that should be evaluated using multiple assessment means.

In the final year (2013-2014), we have obtained a much larger, more reliable temporal network data from Dr. Dimo Dimov at the University of Bath, UK. As noted above, this data set includes 35,757 first-round investments made by 2,498 US-based VC firms between 1980 and 2004, making a total of 24 network snapshots (one for each year).

[Expanding domains of application]

(a) Adaptive network models of social network evolution. Results of computer simulation showed that the relationship between individual agent behavior and several dependent variables, including network centrality, ideational contribution, and ideational interaction strongly depended on a simulation parameter representing the agent's ability to generalize ideas. A transition point for this parameter was found such that centrality relationships observed on either side of the transition point are inverses of each other. The same transition behaviors were also found for other measurements, such as the agent's contributions to idea generation and idea dissemination.

(b) Adaptive network models of corporate merger. Using an agent-based model, we investigated the impact of network structures within and between two merging firms on post-merger cultural integration and organizational dysfunctions—individual turnover, interpersonal conflict and organizational communication ineffectiveness—that arise from insufficient cultural integration. The simulation results demonstrated that the highest level of cultural integration is achieved when social ties are more centralized within each merging firm and the social ties between the merging firms are less concentrated on central individuals. Additionally, the results showed that within-firm and between-firm network structures significantly affect individual turnover, interpersonal conflict and organizational communication ineffectiveness, and that these three outcome measurements do not vary in tandem.
(c) Adaptive network based models of collective behavior of swarms. We applied our automatic equation generating software to analyze the dynamics of collective movements of heterogeneous swarms made of two types analytically. We found that the difference in behavioral traits between the two types tended to increase the local homogeneity within the population. No clear phase transition was detected, however.

(d) Incorporation of GNA into network models of joint technological systems. We analyzed and modeled a real SAR incident in the Arctic that occurred in December 2008. We examined the actual log of inter-agent communications during this SAR incident, and manually reconstructed the rewriting rules that drove the operational network formation. OpNetSim, our simulator software, was then used to simulate the temporal development of the operational network under several hypothetical scenarios. Since the simulation algorithm involves stochasticity, the topology of the simulated network does not exactly match the actual one, but the general trend of increasing agent heterogeneity and concentration on the Search Master node were correctly represented in this model.

(e) Adaptive network models of global state drift in social diffusion. We conducted systematic simulations with the first discrete-time model in which the link replacement probability and the strength of preferential replacement were varied. Results showed that the adaptive link replacement with positive preferential selection caused positive drift of average node states via social diffusion over time. In the final year of the project (2013-2014), we also conducted systematic simulations with the second continuous-time model in which the rates of adaptive link weight adjustment to induce (i) degree-state correlation and (ii) degree disassortativity were varied. Results showed that then the rate for (i) was high, the positive global drift was successfully induced, while the rate for (ii) did not have apparent effects. The proposed approach may be practically implementable in educational settings by, e.g., allowing higher-achieving students to participate in more extracurricular activities.

(f) Adaptive network approach toward distributed self-control of networked dynamical systems. We found that a new second-order control mechanism that uses the difference between the current and desired *directions* of state movement shows much faster, more robust convergence, than the more traditional control mechanism that uses the state difference directly.

**Educational Outreach**

We developed NetSci High: High School Student Research on Network Science, an educational outreach program organized and run in close collaboration with Dr. Stephen Uzzo, Ms. Tara Chudoba and Ms. Catherine Cramer at the New York Hall of Science. This program aims to infuse network science, an emerging interdisciplinary field of study on complex networks, into K-12 education by connecting high school students and teachers to university research labs and letting them work on current network science research for several months, culminating in a poster presentation at NetSci conferences.

In early Fall 2010, we organized initial teachers’ workshops at three locations (New York City, Boston, and Binghamton) to recruit high school science/math teachers and students to this program. The PI attended the New York City workshop and also hosted the Binghamton workshop. As a result,
seven student teams and their teachers participated in the program during 2010-2011 and worked with their local research laboratories. In Binghamton, the PI, Bush and Akaishi collaboratively supervised two student teams (seven female students) in Maine-Endwell high school in Endwell, NY, in close collaboration with Mrs. Julie Gallagher, Assistant Principal of the school.

Each of the seven participating teams worked on its own research project in network science and submitted a poster electronically by mid-April, 2011. The submissions were then reviewed by a scientific committee made of leading network scientists, who selected two winning posters. As a result, four high school students and their teachers (three of them, each representing a different school) traveled to Hungary, Budapest, in June 2011, to participate in the 2011 International Conference on Network Science (NetSci 2011) and present their work there in person. The travel costs were covered by this grant. All of the seven posters were printed and put up at NetSci 2011. Unfortunately none of the Binghamton student teams were selected as winners. The PI later arranged another poster session at the Eighth International Conference on Complex Systems (ICCS 2011) in Boston, MA, for which he served as a Program Chair. Some of the students who could not go to NetSci 2011 were able to come and present their work at ICCS 2011 on their own. At each poster session, the audience was asked to fill in a comment sheet to give encouragement and feedback to the students and teachers who participated in this program.

The second year of the NetSci High program was run as scholarships offered to participating high school student teams. Two student teams participated from the Binghamton area. Due to the shortage of time for program preparation, we could not recruit teams from other areas. The PI supervised one team from Maine-Endwell High School, while another professor in Computer Science at Binghamton University supervised another team from Vestal High School. Those teams were offered a scholarship to attend the NetSci 2012 conference in Evanston, IL, on June 18-22, 2012, and presented their posters to an international audience. For the second year of the program, we also received a corporate donation from BAE Systems. The Maine-Endwell team's research was later put into a journal article and published in PLOS ONE in 2013. This paper attracted a lot of media attention internationally.

We also organized a satellite symposium on education (NetSciEd) at the NetSci 2012 conference. This symposium aimed to address how network science will transform STEM education in the coming years, in anticipation of preparing the next generation of network scientists, as well as addressing the urgent needs in improving STEM education overall. Topics discussed at this event included:
* Network Science in K-16 Practice and Policy
* Network Science in Informal Education
* New Directions in Learning Science
* Developing Metrics for Effective Educational Collaboration Networks

Nine presentations were made by invited speakers who work on the intersection between network science and education. All the presentations are made available publicly on the symposium website. The PI also gave a presentation on his own experience supervising high school students' research projects on networks. At the end of the symposium, a highly active panel discussion was held to determine directions in support of research and
practice in the use of network science to improve education.

After the initial two-year pilot period, NetSci High expanded further as the NSF ITEST project "Network Science for the Next Generation", led by Boston University and the New York Hall of Science. The PI continued to participate in the ITEST project as a consultant.

For the third year of the NetSci High program, the PI supervised one student team from Vestal High School. They participated in a NetSci High summer workshop held at Boston University in the summer of 2012 to learn basics of network science and relevant research methods. They worked with the PI throughout the academic year and prepared a poster by June 2013. Their poster was presented at the NetSci 2013 conference in Copenhagen, Denmark. They also participated in the NetSci High research conference held again at Boston University in the summer of 2013, and presented their project to the audience, including the next cohort of NetSci High participants.

We also organized the second satellite symposium on education (NetSciEd2) at the NetSci 2013 conference. This symposium was organized and hosted in collaboration with the New York Hall of Science. Eleven presentations were made by invited speakers who work on the intersection between network science and education. The PI was a co-organizer of this event.

For the fourth year of the NetSci High program, the PI supervised two student teams from Vestal High School. They participated in the summer workshop at Boston University in the summer of 2013, and then worked on their research projects throughout the academic year. They submitted abstracts to the NetSci 2014 conference as regular submissions. Their submissions were accepted for poster presentations after peer review. The Vestal High School teachers and students conducted a fundraising effort to secure sufficient funding to send all of the eight students and a teacher to Berkeley, CA, where the conference was held. The students participated in the whole conference and presented their posters themselves. They also participated in the NetSci High research conference held at Boston University in the summer of 2014. We also organized the NetSciEd3 symposium at the same conference.

The PI is still continuing his educational outreach partnership with Vestal High School and currently supervising two student teams (eight students, three of whom are female) from Vestal High School. Some of those students attended a regional STEM fair and presented their work to local industry personnel and others involved in the STEM education in the region.

Moreover, the PI organized a regional workshop on K-12 Science Education Outreach at Binghamton University on October 19, 2012, together with Dr. Zhongfei (Mark) Zhang in Computer Science. This workshop aimed to bring all the parties involved in educational outreach activities at Binghamton University and local schools to discuss their approaches, exchange ideas, and brainstorm future developments as a community for engaging the school kids into scientific activities, to serve the ultimate goal of improving and enhancing the K-12 education in this nation in general and in the local community specifically. More than two dozens of panelists participated and had very active and fruitful discussions about educational outreach. For more details, see the workshop website.
* What opportunities for training and professional development has the project provided?

This project provided a number of training and professional development opportunities to all involved, including (1) interdisciplinary graduate training for two graduate research assistants, (2) international research collaboration experience for the PI and the graduate students, and research experience for undergraduate students involved in the project. For more details, please see the "Impact" section.

* How have the results been disseminated to communities of interest?

The outcomes of this project have been disseminated via various channels and integrated in multiple educational programs at Binghamton University and other institutions. The developed algorithms and software tools are made freely available to researchers and other professionals for their own use.

The results of the project have been disseminated through the project websites, publications of journal articles and conference proceedings papers, presentations at conferences and seminars, and other public media channels. Some notable publications include:

- This paper summarizes the overview of the project, describing computational algorithms we developed and applications to social and technological network modeling. It was published last year yet has been cited fourteen times already.

- This paper is an outcome of the NetSci High educational outreach, summarizing the results of the research project by the Maine-Endwell high school students and the PI. This paper has received a tremendous amount of attention from national as well as international media. It has acquired more than fourteen thousand views since its publication.

Also notable are the following two presentation awards that one of the graduate students (Jeffrey Schmidt) and the PI won:

* Best Student Paper Award: Jeffrey Schmidt at IEEE ALIFE 2013

* Best Presentation Award: Hiroki Sayama at IPSJ SIG Mathematical Modelling and Problem Solving in 2010

Finally, some of the project outcomes have been included as instructional materials in the "Dynamical Networks" chapter of the OpenSUNY textbook "Introduction to the Modeling and Analysis of Complex Systems" that the PI is currently writing. This book will be published as an open-access textbook in 2015.

See the "Products" section for more details.
Products

Books

Book Chapters

Conference Papers and Presentations


**Inventions**

**Journals**


**Licenses**

**Other Products**

*Audio or Video Products.*

Several talks related to this project are recorded and posted to the Collective Dynamics of Complex Systems Research Group’s Vimeo channel: http://vimeo.com/user4630872

*Software or Netware.*

[Developing PyGNA]

We developed PyGNA — the Generative Network Automata (GNA) modeling, analysis and simulation framework implemented as a Python module. This framework allows a user to construct adaptive network models based on GNA, either based on the user’s own network rewriting rules or rules that are automatically reconstructed from given network evolution data. The framework also allows dynamic simulations of network behavior.

The first public release version of PyGNA (ver. 0.6) was released in September 2012, and the second public release version (ver. 0.7) was released in August 2013. The third public release version (ver.0.8) was released in December 2014. Its source codes and other information are all publicly available from our SourceForge.net site (ver. 0.6 and 0.7) and github.com (ver. 0.7 and 0.8).

The most recent version (ver. 0.8) of PyGNA has the following capabilities:

(a) Input/output interface of network evolution data. PyGNA can read network evolution data from a file in a GraphML format. GraphML is an XML-based graph mark-up language that can represent multiple graphs in a single file, which we adopted as a general data format to represent time series of networks. PyGNA can also output network time series into a GraphML file.

(b) Identification of network rewriting events and compression of network evolution data. PyGNA can scan a given GraphML file and sequentially detect differences between two consecutive snapshots of networks, and then utilize this information to compress the network evolution data.

(c) Perform a network motif based sampling procedure to identify the distribution of motif transitions, which represent the micro-dynamics responsible for network evolution.

(d) Automatic discovery of subgraph rewriting rules and reconstruction of network evolution. PyGNA can use the
collection of motif transitions generated in (c) above as a set of subgraph rewriting rules and perform network rewritings so as to reconstruct network evolutionary processes from an initial configuration (i.e., simulation of network evolution).

(e) Quantitative evaluation and comparison of the simulated network to the input network to assess the quality of the uncovered dynamics in replicating the input network.

(f) Interactive tutorial written as an executable Python source code file.

**Educational aids or Curricula.**

The PI developed a new graduate-level course "BME-523X: Dynamics of Complex Networks", which was approved by the Binghamton University Graduate Studies Committee and officially ran in Spring 2012. See the attached course syllabus for more details. This course provided students with concepts and mathematical/computational tools of network science, for modeling, analyzing and simulating the dynamics of various complex adaptive networks. Python and NetworkX were used for modeling and analysis of complex networks. The GNA framework was also integrated in the course materials. The course was received very positively by the students and has been approved to be a permanent graduate course by the University. Due to schedule conflicts, this course has not been offered since Spring 2012, but some of the course materials are covered in the PI’s other course (SSIE 523: Collective Dynamics of Complex Systems) in Spring 2013.

**Educational aids or Curricula.**

The PI played a leading role in developing educational materials for the NetSci High students and teachers that have been used at the NetSci High Summer Workshops and other teacher professional development events:
http://www.bu.edu/networks/workshop/

**Organized academic meetings.**

We organized the following meetings:

* STCAN 2010: Special Track on State-Topology Coevolution in Adaptive Networks. This track was held as part of the Fifth International ICST Conference on Bio-Inspired Models of Network, Information, and Computing Systems (BIONETICS 2010), in Boston, MA, on December 1-3, 2010. The track consisted of seven peer-reviewed full papers on various topics relevant to adaptive networks. Dr. Thilo Gross (collaborator for this project) helped organizing this special track as a co-chair, and planned to give a keynote talk. Unfortunately his travel was canceled because of the inclement weather in Europe.

* STCAN 2011: Workshop on State-Topology Coevolution in Adaptive Networks. This workshop was held as part of the Eighth International Conference on Complex Systems (ICCS 2011), in Boston, MA, on June 27, 2011. The workshop hosted seven presentations selected based on abstract reviews. Compared to STCAN 2010, a broader range of application research areas was represented in this workshop, such as management and organizational sciences.

* STCAN 2013: Symposium on State-Topology Coevolution in Adaptive Networks. This symposium was held as a satellite symposium of the 2013 International School and Conference on Network Science (NetSci 2013), in Copenhagen,
Denmark, on June 3, 2013. The event consisted of one keynote talk by Dr. Stefan Bornholdt and 12 contributed talks, which was a significant expansion from the past two STCAN meetings. Dr. Thilo Gross helped organizing this event as a co-chair. This symposium attracted a lot of audience, and the discussions were very active and productive. We believe this event contributed to the development of a research community on adaptive networks significantly.

* NetSci High 2011: International High School Student Poster Competition on Network Science. This new educational outreach program was developed in collaboration with the New York Hall of Science. Two poster sessions were organized: one in the 2011 International School and Conference on Network Science (NetSci 2011), on June 6-10, 2011, Budapest, Hungary, and the other in the Eighth International Conference on Complex Systems (ICCS 2011), Boston, MA, on June 26-July 1, 2011.

* NetSci High 2012: High School Student Research on Network Science. This was a continuation of the NetSci High poster competition organized in the previous year. It was again organized in collaboration with the New York Hall of Science (Dr. Stephen Uzzo and Ms. Catherine Cramer). In 2012, the program was run in the form of scholarships offered to participating high school student teams. Two student teams participated from the Binghamton area. Those teams were offered a scholarship to attend the NetSci 2012 conference in Evanston, IL, on June 18-22, 2012, and presented their posters. One of the students was also invited to give a short oral presentation at the NetSciEd symposium described below. This year, we also received a corporate donation to this program from BAE Systems.

* NetSciEd Satellite Symposium on Education @ NetSci2012: Infuse Network Science into K-12 and Undergraduate Education. This symposium was also organized and hosted in collaboration with the New York Hall of Science. Nine presentations were made by invited speakers who work on the intersection between network science and education. The PI also gave a presentation on his own experience supervising high school students’ research projects on networks.

* Workshop on K-12 Science Education Outreach at Binghamton University. This workshop was organized in October 19, 2012, together with Dr. Zhongfei (Mark) Zhang in Computer Science. It aimed to bring all the parties involved in educational outreach activities at Binghamton University and local schools to discuss their approaches, exchange ideas, and brainstorm future developments as a community for engaging the school kids into scientific activities. More than two dozens of panelists participated and had very active and fruitful discussions about educational outreach.

* NetSci High 2013: High School Student Research on Network Science. Starting this year, the NetSci High program became an NSF ITEST project "Network Science for the Next Generation", led by Boston University and the New York Hall of Science. The PI continued to participate in the ITEST project as a consultant. He also supervised one local student team from Vestal High School. They attended a NetSci High summer camp in 2012 and then presented their year-long research project at a NetSci High conference in the following summer. Their poster was also presented at the NetSci 2013 conference in Copenhagen, Denmark.
* NetSciEd2 Satellite Symposium on Network Science in Education @ NetSci2013. This symposium was also organized and hosted in collaboration with the New York Hall of Science. Eleven presentations were made by invited speakers who work on the intersection between network science and education. The PI was a co-organizer of this event.

* NetSciEd3 Satellite Symposium on Network Science in Education @ NetSci2014. This symposium was also organized and hosted in collaboration with the New York Hall of Science. Nine presentations were made by speakers who work on the intersection between network science and education. The PI was a co-organizer of this event.


Other Publications

Patents

Technologies or Techniques

Thesis/Dissertations

Websites
* Generative Network Automata framework software (PyGNA) on github.com*
https://github.com/schmidtj/PyGNA

NetSci High website
http://tinyurl.com/netscihigh

NetSciEd Symposium website
https://sites.google.com/a/binghamton.edu/netscied12/

NetSciEd2 Symposium website
https://sites.google.com/a/binghamton.edu/netscied2013/

NetSciEd3 Symposium website
https://sites.google.com/a/nyscience.org/netscied3/

Old NetSci High website
https://sites.google.com/a/binghamton.edu/netsci-high-2011-2012/

Project website
http://coco.binghamton.edu/NSF-CDI.html

Workshop on K-12 Science Education Outreach @ BU website
http://bingweb.binghamton.edu/~sayama/K12SEO-BU-workshop.html
Supporting Files

<table>
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<th>Filename</th>
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<tr>
<td>supplemental-documents.pdf</td>
<td>Papers, abstracts, posters etc. produced during 2013-2014</td>
<td>Hiroki Sayama</td>
<td>12/08/2014</td>
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Participants/Organizations

What individuals have worked on the project?

<table>
<thead>
<tr>
<th>Name</th>
<th>Most Senior Project Role</th>
<th>Nearest Person Month Worked</th>
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<tbody>
<tr>
<td>Sayama, Hiroki</td>
<td>PD/PI</td>
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<tr>
<td>Ichinose, Genki</td>
<td>Technical School Faculty</td>
<td>0</td>
</tr>
<tr>
<td>Bush, Benjamin</td>
<td>Graduate Student (research assistant)</td>
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</tr>
<tr>
<td>Schmidt, Jeffrey</td>
<td>Graduate Student (research assistant)</td>
<td>9</td>
</tr>
</tbody>
</table>

Full details of individuals who have worked on the project:

Hiroki Sayama
Email: sayama@binghamton.edu
Most Senior Project Role: PD/PI
Nearest Person Month Worked: 2

Contribution to the Project: The main PI of this project.

Funding Support: One summer month

International Collaboration: Yes, Japan, United Kingdom
International Travel: No

Genki Ichinose
Email: igenki@gmail.com
Most Senior Project Role: Technical School Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Dr. Ichinose was a visiting scholar at the PI’s lab in 2013-2014. He participated in the supervision of two high school student team at Vestal High School.

Funding Support: N/A

International Collaboration: No
International Travel: No

Benjamin James Bush
Email: benjaminjamesbush@gmail.com
Most Senior Project Role: Graduate Student (research assistant)
**Nearest Person Month Worked:** 0

**Contribution to the Project:** Ben worked on computer simulation models of evolving social networks as an application of the adaptive network framework that this project is proposing. He also worked with Jeff on the development of adaptive networks modeling and analysis software.

**Funding Support:** This award (in the past)

**International Collaboration:** No
**International Travel:** No

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**Jeffrey Schmidt**  
**Email:** jschmid1@binghamton.edu  
**Most Senior Project Role:** Graduate Student (research assistant)  
**Nearest Person Month Worked:** 9

**Contribution to the Project:** Jeff worked as a primary developer of the software system this project aims to produce. He went to the NetSci 2014 conference and presented this work. He has also been serving as a graduate student mentor for the Vestal High School student teams.

**Funding Support:** This award

**International Collaboration:** Yes, United Kingdom  
**International Travel:** No

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**What other organizations have been involved as partners?**

<table>
<thead>
<tr>
<th>Name</th>
<th>Type of Partner Organization</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boston University</td>
<td>Academic Institution</td>
<td>Boston, MA</td>
</tr>
<tr>
<td>Chuo University</td>
<td>Academic Institution</td>
<td>Tokyo, Japan</td>
</tr>
<tr>
<td>University of Bristol</td>
<td>Academic Institution</td>
<td>Bristol, UK</td>
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<tr>
<td>University of Connecticut</td>
<td>Academic Institution</td>
<td>Storrs, CT</td>
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<tr>
<td>Vestal High School</td>
<td>School or School Systems</td>
<td>Vestal, NY</td>
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<td>DRDC CORA</td>
<td>Other Organizations (foreign or domestic)</td>
<td>Ottawa, ON, Canada</td>
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<tr>
<td>Maine-Endwell High School</td>
<td>School or School Systems</td>
<td>Endwell, NY</td>
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<tr>
<td>Max Planck Institute for the Physics of Complex Systems</td>
<td>Academic Institution</td>
<td>Dresden, Germany</td>
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<td>Memorial Sloan-Kettering Cancer Center</td>
<td>Academic Institution</td>
<td>New York, NY</td>
</tr>
<tr>
<td>New York Hall of Science</td>
<td>Other Nonprofits</td>
<td>Queens, NY</td>
</tr>
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</table>
Northeastern University  
Academic Institution  
Boston, MA

USMA West Point  
Academic Institution  
West Point, NY

University of Bath  
Academic Institution  
Bath, UK

**Full details of organizations that have been involved as partners:**

**Boston University**

**Organization Type:** Academic Institution  
**Organization Location:** Boston, MA

**Partner's Contribution to the Project:**  
Other: Educational outreach

**More Detail on Partner and Contribution:** The PI collaborated with Dr. H. Eugene Stanley and Dr. Paul Trunfio at Boston University to organize and run the NetSciEd symposia as part of NetSci 2012/2013/2014, as well as to run the NetSci High summer camp at Boston University.

**Chuo University**

**Organization Type:** Academic Institution  
**Organization Location:** Tokyo, Japan

**Partner's Contribution to the Project:**  
Collaborative Research

**More Detail on Partner and Contribution:** Our collaborator Junichi Yamanoi has moved from the University of Connecticut to Chuo University, Tokyo, Japan.

**DRDC CORA**

**Organization Type:** Other Organizations (foreign or domestic)  
**Organization Location:** Ottawa, ON, Canada

**Partner's Contribution to the Project:**  
Financial support  
Collaborative Research  
Personnel Exchanges

**More Detail on Partner and Contribution:** The PI worked with DRDC CORA (Defence Research and Development Canada Centre for Operational Research and Analysis, Ottawa, ON, Canada) under a contract to develop a simulation software that applies the adaptive networks framework to the modeling and analysis of their operational networks for Arctic Search and Rescue (SAR) incidents. This collaboration resulted in one conference paper and one journal paper.

**Maine-Endwell High School**

**Organization Type:** School or School Systems  
**Organization Location:** Endwell, NY
**Partner's Contribution to the Project:**
Collaborative Research
Personnel Exchanges
Other: Educational outreach

**More Detail on Partner and Contribution:** The PI, Bush and Akaishi worked with Mrs. Julie Gallagher, Principal of the Maine-Endwell High School, Mr. John Endress, the School's IT specialist, and two student teams (seven female high school students) on their research projects. This was part of the NetSci-High high school research competition program, which was created and run as part of this grant. The research culminated in two poster presentations that were presented at the 2011 International Conference on Network Science (NetSci 2011) in Budapest, Hungary, as well as at the Eighth International Conference on Complex Systems (ICCS 2011) in Boston, MA. One of the teams continued their research under supervision of the PI and presented another poster at the 2012 International Conference on Network Science (NetSci 2012) in Evanston, IL. Their work was later published in PLOS ONE.

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**Max Planck Institute for the Physics of Complex Systems**

**Organization Type:** Academic Institution
**Organization Location:** Dresden, Germany

**Partner's Contribution to the Project:**
Collaborative Research
Personnel Exchanges

**More Detail on Partner and Contribution:** Dr. Thilo Gross at the Max Planck Institute for the Physics of Complex Systems (MPI-PKS) has been collaborating with the PI. In Summer 2011, Dr. Gross arranged a visiting scholar program at MPI-PKS for the PI and the two graduate students to stay at the Institute and conduct collaborative research. Accommodation and local allowance costs were covered by the Visitors Program of the Institute. The PI and the students were given access to various facilities, including the library and computational resources.

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**Memorial Sloan-Kettering Cancer Center**

**Organization Type:** Academic Institution
**Organization Location:** New York, NY

**Partner's Contribution to the Project:**
Collaborative Research

**More Detail on Partner and Contribution:** We have started a collaboration research project with Dr. Zhirong Bao at MSKCC, on the adaptive network modeling of C. elegans embryogenesis.

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**New York Hall of Science**

**Organization Type:** Other Nonprofits
**Organization Location:** Queens, NY

**Partner's Contribution to the Project:**
Other: Educational outreach

**More Detail on Partner and Contribution:** The PI collaborated with Dr. Stephen Uzzo, Ms. Tara Chudoba and Ms. Catherine Cramer at the New York Hall of Science (NYSci) to organize and run the NetSci-High high school student research program, which was part of this grant. The PI visited NYSci a few times for meetings and hosting
an initial teachers' workshop there. The PI's institution provided funding to NYSci as a participant's cost to fund the NetSci-High program. In 2011, Chudoba and the PI traveled to Budapest, Hungary, to run the high school students' poster session collaboratively. In 2012, Uzzo, Cramer and the PI traveled to Evanston, IL, to run the high school students' poster session collaboratively, as well as to organize the NetSciEd satellite symposium. In 2013, Uzzo, Cramer and the PI traveled to Denmark, Copenhagen, to run the high school students' poster session collaboratively, as well as to organize the NetSciEd2 satellite symposium. In 2014, Uzzo, Cramer and the PI traveled to Berkeley, CA, to organize the NetSciEd3 satellite symposium.

**Northeastern University**

**Organization Type:** Academic Institution  
**Organization Location:** Boston, MA  

**Partner's Contribution to the Project:**  
Facilities  
Collaborative Research  
Personnel Exchanges  

**More Detail on Partner and Contribution:** The PI stayed at the Center for Complex Network Research at Northeastern University during the calendar year of 2014 when he was on sabbatical, and collaborated with Drs. Albert-Laszlo Barabasi and Roberta Sinatra on various projects that are related to this project.

**USMA West Point**

**Organization Type:** Academic Institution  
**Organization Location:** West Point, NY  

**Partner's Contribution to the Project:**  
Other: Educational outreach  

**More Detail on Partner and Contribution:** Mrs. Lori Sheetz at the Network Science Center at USMA West Point helped us in various activities of NetSci High.

**University of Bath**

**Organization Type:** Academic Institution  
**Organization Location:** Bath, UK  

**Partner's Contribution to the Project:**  
Collaborative Research  

**More Detail on Partner and Contribution:** We received a large temporal network data set of the VC investors network from Dr. Dimo Dimov at the University of Bath, UK.

**University of Bristol**

**Organization Type:** Academic Institution  
**Organization Location:** Bristol, UK  

**Partner's Contribution to the Project:**  
Collaborative Research  
Personnel Exchanges
More Detail on Partner and Contribution: Dr. Thilo Gross moved from Max Planck Institute to the University of Bristol, so the PI and his graduate students visited the University of Bristol for research collaboration in summers of 2012 and 2013.

University of Connecticut

Organization Type: Academic Institution
Organization Location: Storrs, CT

Partner's Contribution to the Project:
Collaborative Research

More Detail on Partner and Contribution: The PI collaborated with Dr. Junichi Yamanoi, a former Ph.D. student in the University of Connecticut Business School, to develop a computer simulation model of corporate merger processes represented as an adaptive network. The result was presented at the 2011 International Conference on Network Science (NetSci 2011) in Budapest, Hungary, and also at the Eighth International Conference on Complex Systems (ICCS 2011) in Boston, MA. This collaboration resulted in a few other presentations and a journal article publication.

Vestal High School

Organization Type: School or School Systems
Organization Location: Vestal, NY

Partner's Contribution to the Project:
Collaborative Research
Personnel Exchanges
Other: Educational outreach

More Detail on Partner and Contribution: The PI has been working with Mrs. Carol Reynolds, Computer Science teacher, and Mr. Alan Troidl, Mathematics teacher, both at the Vestal High School, and several student teams on their research projects since 2012. This was part of the NetSci-High high school research program, which was created and run as part of this grant.

Have other collaborators or contacts been involved? No

Impacts

What is the impact on the development of the principal discipline(s) of the project?

This project has produced a novel theoretical framework and a computational toolkit that are expected to become the basis of transformational ways of studying the coevolution of dynamics on and of complex networks, and thereby achieve significant advances in the modeling and prediction of their temporal evolution.

What is the impact on other disciplines?

The outcomes of this project will be useful in many cutting-edge fields, including social network science, organizational research, network ecology and epidemiology, systems biology, bioinformatics, and many others. Areas of
application include social network analysis, modeling and analysis of organizational behavior, and modeling and analysis of biological network formation. The developed framework will also serve as a generalized conceptual/mathematical 'language' for modeling, analyzing and discussing the dynamics of various complex systems, which will galvanize interdisciplinary discussion and collaboration across many different areas of applications. To facilitate cross-disciplinary discourses, international workshops/special sessions have been organized several times already.

What is the impact on the development of human resources?

Through collaboration with Dr. Thilo Gross at the University of Bristol (formerly at the Max Planck Institute for the Physics of Complex Systems), the PI has acquired mathematical knowledge and skills for analytical study of adaptive network dynamics using moment closure techniques, as well as many creative ideas and insights into how one could effectively represent and analyze various dynamics of adaptive networks.

This project involved two graduate research assistants (Jeff Schmidt and Benjamin James Bush). Bush joined in Fall 2010 and has worked on the application of adaptive networks to social network modeling and analysis. He is from an underrepresented group (Hispanic). Schmidt joined in Spring 2011 and has been the main software developer of PyGNA, working on the implementation of the GNA framework in Python/NetworkX. Both students enrolled in the Ph.D. program in Systems Science at Binghamton University, and the PI supervised their work. Both students took a graduate course on computational modeling taught by the PI.

The two graduate students received multidisciplinary research training under financial support from this NSF award, including international collaboration with Dr. Thilo Gross at the University of Bristol, UK (formerly at the Max Planck Institute for the Physics of Complex Systems in Dresden, Germany) in the summer of 2011, 2012 and 2013. The PI and the graduate students (both in 2011 and 2012; only Schmidt in 2013) stayed in Dr. Gross’s lab during the summers and had intensive discussions with him as well as his staff. Schmidt also accompanied the PI in his visit to DRDC-CORA in Ottawa, Canada, in September 2011, and participated in the initial stage of the collaboration with DRDC-CORA.

Schmidt has obtained a Master’s degree for his research on this project in Fall 2012. A conference paper based on his Master’s thesis won the Best Student Paper award at the IEEE Symposium on Artificial Life in April 2013. Both students are currently working on journal articles that summarize their research outcomes, as well as writing their respective PhD dissertations.

In addition, the PI, Bush, Schmidt, Jin Akaishi (collaborator) and Genki Ichinose (collaborator) participated in the supervision of local high school student teams through the NetSci High program. They had weekly meetings with two student teams on a regular basis to discuss research progresses, tasks and directions. They all gained valuable educational experiences through these outreach activities. The PI continues supervising various high school student teams to date.
This project also involved several undergraduate assistants. Steven Krell (Bioengineering junior) was hired to assist the PI in organizing the STCAN 2011 workshop and the ICCS 2011 conference itself (for which the PI served as a Program Chair). While he did not conduct any research, Krell was able to attend the workshop/conference as a staff member and learned a lot about complex systems and network sciences. For research, Chun Wong (Bioengineering senior) was hired during Spring 2012 to help the PI develop the simulation software for the collaboration project with DRDC-CORA. He accompanied the PI and Schmidt in their visit to DRDC-CORA in Ottawa, Canada, in September 2011. Finally, Alex Hantman (Bioengineering junior) helped writing prototype codes for the collaboration project with Dr. Zhirong Bao during summer 2012.

**What is the impact on physical resources that form infrastructure?**
Nothing to report.

**What is the impact on institutional resources that form infrastructure?**
The new graduate course on complex adaptive networks produced in this project will serve as an educational resource for faculty and students at Binghamton University.

**What is the impact on information resources that form infrastructure?**
This project is producing PyGNA, a free software package of the GNA framework for modeling and analysis of complex adaptive networks, which will be a useful computational resource for broader research communities.

Moreover, the educational outreach program developed as part of this project, NetSci High, has come to be recognized very positively among the international network science community. It will serve as a continuing educational resource for those who want to initiate similar K-12 outreach programs that will bridge secondary education with cutting-edge scientific research labs.

**What is the impact on technology transfer?**
The software developed in this project is made publicly available from SourceForge.net and github.com. No technology transfer related action was taken yet.

**What is the impact on society beyond science and technology?**
The proposed GNA framework may help model and understand many real-world social/organizational/operational networks, which may help better inform policy makers and business practitioners. For example, we collaborated with DRDC CORA on GNA-based modeling of their operational networks. The outcome of this project may inform Canadian Defence authorities about what kind of organizational improvements will help make their SAR response joint systems more efficient. Similarly, our recent work on cultural integration after corporate merger may offer many valuable implications for how to make corporate M&A effective and successful.

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**Changes/Problems**
Changes in approach and reason for change
Nothing to report.

Actual or Anticipated problems or delays and actions or plans to resolve them
Nothing to report.

Changes that have a significant impact on expenditures
Nothing to report.

Significant changes in use or care of human subjects
Nothing to report.

Significant changes in use or care of vertebrate animals
Nothing to report.

Significant changes in use or care of biohazards
Nothing to report.