Siemens Competition
Math : Science : Technology
Regional Finalist

Name: Ryan Catalano
High School: North Brunswick Township High School
Mentor: Matthew Lucia, Princeton University
Project Title: *Characteristics of a Two-Grid Inertial Electrostatic Confinement (IEC) Fusion Device Operating at High Pressure*

The long sought after goal of magnetic and inertial fusion research is to make net energy. One unique confinement scheme, Inertial Electrostatic Confinement (IEC), would potentially allow for compact, cost-effective reactors in the future. Small IEC neutron generators that exist today could be used in applications such as explosives detection, cancer treatment, and isotope production. Typical machines based on IEC operate at pressures below 10 mTorr and the effects of voltage and current have been well studied. The interactions between voltage and pressure have yet to be analyzed for a device that operates out of this range with a small electrode spacing (less than 2 cm). The operating characteristics of an IEC fusion device were examined under varying operating conditions as defined by a two-level full factorial experimental design. Tests were conducted at pressures ranging from 25.0 mTorr to 29.1 mTorr. The result was a mathematical model that showed a statistically significant interaction between deuterium pressure and applied voltage — at higher pressure the same change in applied voltage produced a greater effect on the neutron output. The experiments also demonstrated that neutron flux was strongly dependent on the current.

Siemens Competition
Math : Science : Technology
Regional Finalist

Names: Emily Cheng, Kelly Jiang & Gerald Liu
High Schools: Methacton High School & Conestoga High School
Mentor: Ying-Hsiu Su, Baruch S. Blumberg Institute
Project Title: *Simultaneous Detection of Genetic and Epigenetic DNA Modifications by Targeted Next Generation Sequencing for Cancer Screening --Assay and Data Analysis Software Development for the Detection of Hepatocellular Carcinoma*

Hepatocellular Carcinoma (HCC) is the third leading cause of cancer mortality in the United States with over 24,000 deaths annually. Due to heterogeneity of HCC, a single marker is unlikely to have sufficient sensitivity for screening. In this study we developed an assay for simultaneous detection of a panel of five genetic and epigenetic DNA modifications for HCC screening in urine by utilizing Next Generation Sequencing's (NGS) high through-put and multiplex capability. The two major limitations of NGS are the inherent error rate of 2-3% and the bottleneck of data analysis. To enhance the sensitivity of NGS in detecting mutations or methylations to 0.1 % sensitivity, we used locked or bridged nucleic acid (LNA or BNA) to suppress the wild-type templates and enrich the mutated sequence, also designed unique bisulfite specific primers in the regions that contain CpG sites for methylation detection. In order to facilitate the data analysis of millions of DNA sequencing reads, a novel software tool was developed to efficiently detect and extract mutation and methylation information of interest of the tested genes. In this study, the sensitivity improvement was validated by Sanger sequencing analysis of reconstituted standards. By using a pilot NGS data, we showed that the software was efficient and accurate in analyzing the data, thus reducing the analysis time required from 8 hours to 5 min (~100-fold reduction). The assay was then applied to 46 archived HCC patient urine DNA samples and submitted to NGS. This is the first study to successfully simultaneously detect cell-free circulating genetic and epigenetic DNA modifications using targeted NGS technology and our newly developed customizable software (fastNGSDetect) for data analysis. This method can be applied to the detection of other mutated and methylated DNA biomarkers, for other cancer detection and liquid biopsy for precision medicine to improve cancer patient care. .

Siemens Competition
Math : Science : Technology
Regional Finalist

Names: Thomas Choi & Matthew Wang
High Schools: Phillips Academy & Princeton High School
Mentor: Charles Hailey, Columbia University
Project Title: *An X-ray Search for Evidence of Black Hole Settling in the Galactic Center by Dynamical Friction*

We analyze a decade's worth of data in M.P. Muno's X-ray Chandra catalog of 9017 galactic center sources in an attempt to find black hole low-mass X-ray binary system clustering towards the galactic center. Because the Central Hard X-ray Emissions (CHXE) of 8 x 4 parsecs is believed to consist mostly of intermediate polars, we analyze the more massive black hole binary candidates with the less massive intermediate polar candidates in one-dimensional and two-dimensional spatial morphology. Within the central 1 - 2 parsecs of the galaxy, the black hole binary candidates show definite cusping towards the galactic center, whereas the intermediate polar systems yield a more extended distribution. These results are the first observational evidence in over 30 years to support the theory of dynamical friction and they offer significant initial research for galactic center astrophysics.

Siemens Competition
Math : Science : Technology
Regional Finalist

Names: Fengyao Ding & Cristian Gutu
High Schools: Phillips Academy & Joel Barlow High School
Mentor: Young Hyun Kwon, Massachusetts Institute of Technology
Project Title: *SecretRoom: An Anonymous Chat Client*

While many people would like to be able to communicate anonymously, the few existing anonymous communication systems sacrifice anonymity for performance, or vice-versa. The most popular such app is Tor, which relies on a series of relays to protect anonymity [17]. Though proven to be efficient, Tor does not guarantee anonymity in the presence of strong adversaries like ISPs and government agencies who can conduct in-depth traffic analysis.

In contrast, our messaging application, SecretRoom, implements an improved version of a secure messaging protocol called Dining Cryptographers Networks (DC-Nets) to guarantee true anonymity in moderately sized groups [11]. However, unlike traditional DC-Nets, SecretRoom does not require direct communication between all participants and does not depend on the presence of honest clients for anonymity. By introducing an untrusted server that performs the DC-Net protocol on behalf of the clients, SecretRoom manages to reduce the O(n2) communication associated with traditional DC-Nets to O(n) for n clients. Moreover, by introducing artificially intelligent clients, SecretRoom makes the anonymity set size independent of the number of “real” clients. Ultimately SecretRoom reduces the communication to O(n) and allows the DC-Net protocol to scale to hundreds of clients compared to a few tens of clients in traditional DC-Nets.

Siemens Competition
Math : Science : Technology
Regional Finalist

Names: John Heath, JunHyuk Oh & Emma Winson
High Schools: South Pasadena High School & The Hockaday School
Mentor: Young Hyun Kwon, Massachusetts Institute of Technology
Project Title: *Utilizing an All Synthetic Epitope Targeting Strategy to Develop Potential Inhibitors against Allosteric Sites on the Oncoprotein KRas*

We utilized a synthetic epitope targeting strategy to discover binders against allosteric sites on the protein KRas. KRas, when mutated, constantly signals for cell division, therefore promoting tumorigenesis. Our binder, called a Protein Catalyzed Capture (PCC) Agent, mimics the behavior of an antibody developed against KRas, but unlike antibodies, is also capable of reaching KRas within the cytoplasm of a cell. We synthesized a small fragment of KRas (the epitope), but modified to present an azide click handle. That epitope was incubated with a bead-based library of 2 million alkyne-presenting cyclic peptides. Under conditions of the screen, if the epitope and library element bind in just the correct orientation, the azide and alkyne groups "clicked," together, forming a covalent (triazole) bond. This covalent bond defined a bead as a "hit." The peptides on hit beads were sequenced by Edman degradation, and two proposed binders were scaled up and tested in an immunoassay against the full length KRas protein. We conclude with the development of a binder to KRas with an affinity or EC50 value of 1.7±.68μM, and furthermore, since the epitopes chosen were allosteric sites of KRas, it can stated that the ligands are drug candidates.

Siemens Competition
Math : Science : Technology
Regional Finalist

Name: Milind Jagota
High School: Liberty High School
Mentor: Melissa Waldron, Liberty High School
Project Title: *Computational Study of Random Nanowire Networks: Optimization of Conductivity through Orientation*

Transparent conductors are ubiquitous in modern electronic devices. The majority of devices use Indium Tin Oxide (ITO) for this purpose. ITO, however, is plagued by issues including material scarcity, high manufacturing costs, and brittleness. Random metal nanowire films show potential as transparent conductors, but their performance must be improved before large-scale displacement of ITO can occur. In this study, nanowire orientation was investigated as a method for optimizing performance of random metal nanowire films. A computational model was developed to generate random nanowire networks and calculate their electrical conductivity. The model was then used to investigate the effects of nanowire orientation on network conductivity using three different distributions: normal, uniform, and discrete bimodal. For all three, conductivity is maximized for an optimal degree of restriction, corresponding to standard deviations of 35°, 33°, and 21°, respectively. For the first two distributions, conductivity increases with respect to the isotropic control by 25% and 20%, respectively. Surprisingly, the bimodal distribution showed no such enhancement, emphasizing the crucial role of randomness in orientation effects. These results are expected to support wider adoption of metal nanowire networks as transparent conductors, which will reduce costs and accelerate development of electronic devices.

Siemens Competition
Math : Science : Technology
Regional Finalist

Names: Kwonil Ko & Seung Hwan An
High Schools: Cushing Academy & Taft School
Mentor: Dan Ismailescu, Hofstra University
Project Title: *Avoiding Monochromatic Configurations In The Multi-colored Plane*

Given an integer $r \geq 2$, an *r-coloring* of the plane is a partition of the 2-dimensional Euclidean space into r classes. Let K be a finite point set in the plane. For a given r-coloring, we say that color i *avoids* K, if no congruent copy of K has all points of the i-th color. In particular, if K consists of two points distance d apart, we simply say that color i avoids distance d.

In this paper we prove the following results:

- There exists a 3-coloring of the plane, and a 6-point configuration P such that two of the colors avoid distance 1, and the third color avoids P.
- There exists a 4-coloring of the plane, and a 4-point configuration Q such that three of the colors avoid distance 1, and the fourth color avoids Q.
- There exists a 5-coloring of the plane, and a 3-point configuration T such that four of the colors avoid distance 1, and the fifth color avoids T.

Siemens Competition
Math : Science : Technology
Regional Finalist

Name: Kunal Singh
High School: High Technology High School
Mentor: Dimitris Samaras, Stony Brook University
Project Title: *Classification of Subtle Morphological Features for Individual Nuclei in Stained Glioma Tissue Slides*

Gliomas are one of the most complex and deadly types of brain cancers that affect millions of people worldwide. Pathologists diagnose different types of glioma by analyzing the visual features of nuclei in stained tissue samples from biopsies. However, due to the high number of nuclei present on a whole slide image, it is difficult to characterize all of the nuclei manually. This paper presents a novel framework for the automatic classification of shapes and multiple attributes for individual nuclei in glioma tissue slides. A set of six target classes based on shape and a set of nine target classes based on attributes were established. 1650 separate images of nuclei from both low-grade glioma and high-grade glioma tissue slides were annotated with a single descriptive shape class and multiple descriptive attributes classes. Nuclei images were segmented using color deconvolution and image enhancement, and Local Binary Patterns and Gabor filter responses were extracted as representative features. Multiple shape and attribute Support Vector Machine (SVM) models were trained with subsets of the feature sets using an RBF-kernel and optimized parameters with 5-fold cross validations. The shape SVM models were designed to predict a single shape class for a given instance while the attribute models were designed to predict multiple attribute classes. The average weighted classification pre-cision for shapes was 71.18% and the jaccard similarity score for attributes was 74.90% for a 200-image test set. This work is the first to classify two types of subtle morphological nu-clei features in a separate manner. Additionally, our framework for classification is generic and can be applied to other pathology image classification problems. Through a framework to automatically classify both shapes and attributes separately, pathologists will have richer information to make more informed diagnoses about the type of glioma is present in a certain tissue sample.

Siemens Competition
Math : Science : Technology
Regional Finalist

Name: Konrad Urban
High School: Fox Chapel Area High School
Mentor: Justin Patterson, Fox Chapel Area High School
Project Title: *Improving Quality of Service Protocols With Genetic Multi-Swarm Particle Swarm Optimization Algorithm*

As computer networks grow larger and more complex, receiving communications quickly and with low error is becoming imperative for financial systems, military net-works, and commercial applications. Network engineers provide limited guarantees about latency, error rate, and other network properties by imposing Quality of Service (QoS) constraints on certain network properties. Finding the lowest-cost networking route which meets QoS constraints is a NP Complete problem, so shortest-path al-gorithms working in polynomial time will not reliably find the best solution while meeting QoS constraints. Swarm algorithms, which stochastically search a solution space based on the optimization behaviors of biological swarms, have been success-fully applied to the QoS constrained routing problem. I consider the performance of a variant on Particle Swarm Optimization (PSO) called Multi-swarm Particle Swarm Optimization (MPSO). I integrate MPSO with a genetic rule to improve on existing al-gorithms' performance. I propose a multicast routing algorithm called Genetic MPSO (GMUPSO) for improving QoS routing protocols. I hypothesize that GMUPSO will construct routes with lower latency than two standard and effective QoS routing algo-rithm. By evaluating my algorithm in a simulation environment, GMUPSO validates my hypothesis by outperforming the existing algorithms in creating paths with lower average latency and in other metrics.

Siemens Competition
Math : Science : Technology
Regional Finalist

Name: Ziheng Wang
High School: Saint Paul's School
Mentor: Carlos Simmerling, Stony Brook University
Project Title: *High Throughput Drug Design by a Novel Grid-based Computational Method*

Current free energy calculation methods like MM-GBSA and FEP require new molecular dynamics simulations for each ligand considered, making them too expensive for routine application in lead optimization settings. To address the unfavorable computational cost scaling, a grid-based method, OWFEG-GB (One Window Free Energy Grid-Generalized Born), was developed. Ensemble averaged free energy grids are generated from a molecular dynamics simulation trajectory of the protein-drug complex. An implicit solvent model is used to account for desolvation effects. Once the grids have been generated, the effect of each new chemical modification on the binding free energy of the drug can be scored in a matter of seconds. OWFEG-GB scores were found to outperform or match MM-GBSA results in predicting experimental binding free energy values, even when difficult effects such as binding mode variation and induced fit were considered. The grids can also be directly visualized to locate potential beneficial modifications, an important functionality unavailable in typical free energy calculation methods. In addition, OWFEG-GB was used to successfully identify potential targetable allosteric binding pockets on H-Ras. These promising results indicate OWFEG-GB has the potential to be developed into a useful tool for all stages of rational drug discovery and design.