**Title:** Real-time inventory of computational resource utilization for de novo assembly of microbial genomes with PacBio and Illumina reads

**Abstract:** De novo assembly of finished microbial genomes benefits equally from the read quality and length afforded by the Illumina and PacBio platforms, respectively, but each chemistry introduces inherently different computational challenges for genome reconstruction. We evaluated computational resource utilization on an Amazon EC2 instance running the hierarchical genome assembly process (HGAP) for PacBio-only assembly in comparison to several short-read-only and hybrid assemblies using existing MSI resources, and we show that closed microbial genomes are achievable with comparable computational resources already available at MSI.

**Lead author:** Jon Badalamenti

**MSI Principal Investigator:** Daniel Bond (Biotechnology Institute)

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**Title:** Family conflict and neural activity during self processing in depressed adolescents

**Abstract:** The objective of the project was to determine if family conflict contributes to certain behaviors related to depression. The second objective was to determine whether certain structures of the brain are activated when adolescents with family conflicts think about themselves from different points of view and how that may be correlated to their depression.

**Lead author:** Jonathan Batres

**MSI Principal Investigator:** Karina Quevedo (Psychiatry)
Title: High-performance de novo RNA-transcript reconstruction leveraging distributed memory and massive parallelization

Abstract: Exemplifying collaborative software development between industry and academia to tackle computational challenges in manipulating large volumes of next-gen sequence data, leveraging advances in algorithm development and compute hardware, we describe our efforts to optimize the performance of the Trinity RNA-Seq de novo assembly software. Three versions of Trinity's Inchworm computationally intensive part (one that is based on the original OpenMP version, and two new versions that are based on MPI and on Fortran2008) are integrated into the Galaxy web interface, with jobs running on a Cray XC30.

Lead author: Pierre Carrier

MSI Principal Investigator: Carlos Sosa (BICB - UM Rochester)

Title: Pathophysiology of spasmodic dysphonia: A combined TMS and fMRI study

Abstract: In this poster, we will present our preliminary data (two healthy controls) of the pathophysiology of spasmodic dystonia study. We used: FSL, AFNI and Matlab software package on “Itasca” (MSI supercomputer) to process the fMRI image data and calculate the relationship between TMS hotspot and fMRI activation areas of two different tasks. We also used JMP on “Copper” (MSI supercomputer) to do the statistical analysis.

Lead author: Mo Chen

MSI Principal Investigator: Teresa Kimberley (Physical Medicine and Rehabilitation)
Title: Optimal algorithm for metabolomics classification and feature selection varies by dataset

Abstract: A systematic comparison of commonly used algorithms on synthetic and empirical metabolomics datasets of different sample size and number of classes.

Lead author: Charles Determan

MSI Principal Investigator: Greg Beilman (Surgery)

Title: Mining predictive and interpretable patterns from electronic health record

Abstract: We aim at finding patterns from electronic health records that can predict a clinical outcome and simultaneously be interpretable to domain experts.

Lead author: Sanjoy Dey

MSI Principal Investigator: Vipin Kumar (Computer Science and Engineering; MSI Fellow)
Title: Hippocampal volumetric analysis of mucopolysaccharidosis I

Abstract: We are currently investigating whether or not hippocampal subdivision volumes (namely that of the head, body, and tail) are related to verbal and nonverbal memory in healthy and MPS I subjects. Such comparisons between MPS I and healthy subjects will further provide insight into the cognitive implications of brain differences.

Lead author: Gabriel Garcia-Paredes

MSI Principal Investigator: Elsa Shapiro (Pediatrics)

Title: Inferring gene regulatory networks in cardiac differentiation by integrating RNA-seq and ChIP-seq data

Abstract: Heart development during lineage commitment are coordinated by precise temporal regulation of thousands of genes. Based on recently published data on massively parallel sequencing for several histone modifications (H3K4me3, H3K4me1, H3K27me3 and H3K27ac), RNA polymerase II binding sites, and gene expression levels at mouse embryonic stem cells (ESCs), mesoderm, cardiac precursors and cardiomyocytes, we developed a novel and efficient algorithm to reconstruct regulatory networks by integrating temporal multi-view biological information.

Lead author: Wuming Gong

MSI Principal Investigator: Daniel Garry (Medicine)
Title: Characterization of human intestinal fungal communities using a validated, combined qPCR-targeted sequencing strategy

Abstract: Research combines next-generation sequencing with a validated qPCR approach to study the human intestinal fungal microbiome in a neonatal population. The focus of the research is on studying the diversity of the fungal microbiomes from different donors and elucidating differences linked to age and disease state.

Lead author: Tim Heisel

MSI Principal Investigator: Cheryl Gale (Pediatrics)

Title: Docking simulation and molecular mechanics calculation of relative binding free energy of ouabain, its analogues, and cetirizine to investigate the basis for their selectivity toward the Na,K-ATPase α4 isoform

Abstract: Ouabain, its analogues (SS-I-24, SS-I-42, and SS-I-54), and cetirizine exhibit good isoform selectivity toward the α4 isoform of Na,K-ATPase over the α1 isoform of the enzyme. We employed the computational methods to investigate their selectivity toward the Na,K-ATPase α4 isoform.

Lead author: Kwon Ho Hong

MSI Principal Investigator: Gunda Georg (Institute for Therapeutics Discovery and Development)
Title: Neurobiological impact of pubertal development during social ostracism and self-facial recognition in depressed adolescents

Abstract: The poster will include findings from fMRI tasks that examined the difference in brain activity between depressed and healthy adolescents when they engaged in a social exclusion paradigm and a facial recognition paradigm. Our preliminary results show that healthy adolescent who are in later pubertal stage have greater activation in hippocampus than depressed adolescent with the same pubertal stage when they engaged in facial recognition. However, increased activities in anterior cingulate cortex and amygdala were shown as puberty progressed in depressed adolescents when they were socially excluded.

Lead author: Yeonjin Kim

MSI Principal Investigator: Karina Quevedo (Psychiatry)

Title: Computational, synthetic, biochemical and structural biology methods for anthrax toxin lethal factor (LF) inhibitor design

Abstract: Anthrax presents a significant threat to society as a bioterrorism agent. The lethal factor (LF) enzyme secreted by B. anthracis is chiefly responsible for anthrax-related cytotoxicity and eventual host death. In this poster, we present the modeling, synthesis, experimental evaluation, and structural biology studies of compounds that are specifically designed to explore the key S2’ LF binding region, in order to obtain design principles for hit-to-lead optimization of small-molecule anti-anthrax therapeutics.

Lead author: Elbek Kurbanov

MSI Principal Investigator: Elizabeth Amin (Medicinal Chemistry)
Title: SHEAR: Sample heterogeneity estimation and assembly by reference

Abstract: Analysis of next-generation sequence data from tumor tissue samples is made difficult by computational challenges related to intra-tumor heterogeneity and highly mutated tumor genomes. We developed SHEAR, an analysis tool that tackles some of these challenges by accurately and efficiently detecting structural variation, generating personal genomic sequences for downstream analyses, and accounting for heterogeneous sequencing samples by estimating the subpopulation/subclone percentage for each heterogeneous variant.

Lead author: Sean Landman

MSI Principal Investigator: Vipin Kumar (Computer Science and Engineering; MSI Fellow)

Title: Single-cell RNA-seq insights into global gene expression changes in RDEB patients

Abstract: This pilot experiment seeks to develop a pipeline for the analysis of single-cell RNA-seq data using recessive dystrophic epidermolysis bullosa (RDEB) patients and their sibling matched normals to look at global changes in gene expression and variation among individual cells.

Lead author: Catherine Lee

MSI Principal Investigator: Jakub Tolar (Pediatrics)
Title: Global effects on transcriptome of the essential protein Gcp of *Staphylococcus aureus*

Abstract: The conserved protein Gcp is essential for bacteria growth; however, its essential mechanism remains unclear. In this study, we utilized the next generation RNA-seq technology to determine the effect of depletion of Gcp on global gene transcription in *Staphylococcus aureus* and identified many operons that were dramatically affected, providing fundamental information to elucidate essential function of Gcp.

Lead author: Ting Lei

MSI Principal Investigator: Yinduo Ji (Veterinary and Biomedical Sciences)

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Title: Mutation of the ovarian cancer genome by APOBEC3B

Abstract: Using both cell based and bioinformatic approaches, we have identified APOBEC3B as a significant source of mutation in ovarian cancer. These data suggest a model in which APOBEC3B drives tumor evolution and provide precedent for the use of APOBEC3B as a novel target for ovarian cancer therapies.

Lead author: Brandon Leonard

MSI Principal Investigator: Reuben Harris (Biochemistry, Molecular Biology, and Biophysics)
Title: Fast, fully Bayesian spatiotemporal inference for fMRI data

Abstract: We implement a spatiotemporal model on a massive neuroimaging dataset using a dimension reduction technique that allows for an embarrassingly parallel implementation resulting in greater computational efficiency over previous methods. We demonstrate the effectiveness and suitability of our model via a simulation study and by analyzing fMRI data from the Minnesota Twins Study.

Lead author: Donald Musgrove

MSI Principal Investigator: John Hughes (Biostatistics)

Title: Orientation of TOAC-spin-labeled phospholamban studied by MD simulation and EPR spectroscopy

Abstract: Phospholamban (PLB) is a small membrane protein that regulates calcium uptake into the sarcoplasmic reticulum in cardiac cells by inhibiting the CA2+-ATPase (SERCA). Molecular dynamics (MD) simulation of PLB with a rigidly attached spin label, TOAC, is carried out to elucidate orientations of PLB's secondary structural elements and TOAC orientation in relation to the membrane with the aim to assist interpretation of EPR data.

Lead author: Andrew Reid

MSI Principal Investigator: David Thomas (Biochemistry, Molecular Biology, and Biophysics; MSI Fellow)
**Title:** Nano-engineered mesenchymal stem cells as targeted therapeutic carriers

**Abstract:** We used nano-engineered mesenchymal stem cells (MSCs) as tumor-targeted therapeutic carriers. We hypothesized that incorporation of drug-loaded, polymeric nanoparticles in MSCs will allow for tumor-targeted and sustained drug delivery. Our studies demonstrate that nano-engineered MSCs can be loaded with high concentration of anticancer agents without affecting their migratory or drug resistance potential.

**Lead author:** Tanmoy Sadhukha

**MSI Principal Investigator:** Swayam Prabha (Pharmaceutics)

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**Title:** Visualization and quantification of high-resolution 4-dimensional blood flow in the human brain and aorta using 7 tesla ultra-high field magnetic resonance imaging

**Abstract:** The Center for Magnetic Resonance Research at the University of Minnesota hosts 2 of worldwide ~40 ultra-high field (7 Tesla) human magnetic resonance imaging (MRI) scanners, which allow higher spatial resolution, faster acquisition, and stronger image contrast compared to clinical MRI systems. The poster will illustrate how we utilize this system to measure the human blood flow in the brain and in the aorta with high spatial and temporal resolution (i.e., 4-dimensional) and how we use dedicated tools provided by MSI to visualize, analyze, and quantify this information.

**Lead author:** Sebastian Schmitter

**MSI Principal Investigator:** Pierre-Francois van de Moortele (Center for Magnetic Resonance Research)
Title: Impulsivity, adolescence, and reward-related brain activation: An MZ twin fMRI study

Abstract: In this poster, I hypothesize that reward-related brain activation (BOLD signal) during the monetary incentive delay task in regions of interest (such as the ventral and dorsal striatum) will be correlated with trait impulsivity (measured using the MPQ; Multidimensional Personality Questionnaire). Using MZ twins, we tested the genetic and environmental contributions to this relationship.

Lead author: Merav Silverman

MSI Principal Investigator: Kathleen Thomas (Institute of Child Development)

Title: FRET-based trilateration of a domain peptide bound within functional ryanodine receptors

Abstract: The ryanodine receptor (RyR) Ca2+ triggers muscle contraction by releasing Ca2+ from the sarcoplasmic reticulum. Trilateration based on confocal FRET measurements, simulated annealing calculations on fluorescent labeled proteins, and X-ray crystallography and cryo-electron microscopy structural data was used to determine the location of the DPc10 modulatory interface within the ryanodine receptor channel.

Lead author: Bengt Svensson

MSI Principal Investigator: David Thomas (Biochemistry, Molecular Biology, and Biophysics; MSI Fellow)
Title: Amygdalar volumes and acquired autism in MPS IIIA (Sanfilippo Type A Syndrome)

Abstract: Purpose: To compare differences in amygdalar volumes between autistic, and non-autistic Cross-sectional Study. Use of MSI resources in the analysis of human brain MRI scans individuals with MPS IIIA. MPS IIIA is a progressive, neurodegenerative, lysosomal disorder with severe cognitive and behavioral impairment. (1) Amygalae: Using manual segmentation with BRAINS2 (Brain Research: Analysis of Images, Networks, and Systems). (2) Total brain (cortical and intracranial): Using automated segmentation with FreeSurfer software. (3) Shape analysis to render 3D volumes of the amygdala with Avizo software

Lead author: Amy Wakumoto

MSI Principal Investigator: Elsa Shapiro (Pediatrics)

Title: Differential analysis techniques for comparing contrasting diabetes patients

Abstract: Diabetes is reaching pandemic levels in the United States (U.S.), affecting around 8-9% of the total U.S. population. The availability of de-identifiable electronic health records (EHR) provides an opportunity to study the prevalence of diabetes among subgroups (based on gender, race, age, economic disparities) of human population. Use of differential analysis techniques to identify emerging patterns among diabetes patients will lead to improvement in evidence based practice guidelines.

Lead author: Pranjul Yadav

MSI Principal Investigator: Vipin Kumar (Computer Science and Engineering; MSI Fellow)
Title: Evaluating climate models on their ability to replicate climate teleconnections

Abstract: Climate teleconnections reflect an important aspect of variability in atmospheric circulation. We propose different methodologies to evaluate the different Global Circulation Models (GCM’s) on their ability to replicate EnSO (El-Nino Southern Oscillation)- a well-known climate teleconnection that highly impacts the climate of different regions around the world.

Lead author: Saurabh Agrawal Airan

MSI Principal Investigator: Vipin Kumar (Computer Science and Engineering; MSI Fellow)

Title: L2AP: Fast cosine similarity search with prefix L-2 norm bounds

Abstract: In the context of cosine similarity and weighted vectors, leveraging the Cauchy-Schwarz inequality, we propose new L2-norm bounds for reducing the inverted index size, candidate pool size, and the number of full dot-product computations for solving the All-Pairs similarity search, or self-similarity join, problem. Our new pruning strategies enable significant speedups over baseline approaches, most times outperforming even approximate solutions.

Lead author: David Anastasiu

MSI Principal Investigator: George Karypis (Computer Science and Engineering)
Title: First principles simulations of Objective Structures

Abstract: We describe the development and implementation of quantum mechanical simulation methods for atomic/molecular structures with high symmetries called Objective Structures. We mention how this work has been leading to new approaches for first principles nanomechanics simulations as well as to the discovery of novel materials.

Lead author: Amartya Banerjee

MSI Principal Investigator: Ryan Elliott (Aerospace Engineering and Mechanics)

Title: Extracting structural and mechanical properties of lipid vesicles from molecular dynamics simulations

Abstract: We have developed a novel method using spherical harmonic analysis to characterize the structure and mechanical properties of lipid vesicles from molecular dynamics simulation.

Lead author: Anthony Braun

MSI Principal Investigator: Jonathan Sachs (Biomedical Engineering)
Title: Information-theoretic analysis for crowd motion prediction

Abstract: Crowd simulation techniques’ performances vary under different scenarios and an information theoretic measurement called Entropy Metric can be used to compare the simulator’s similarity with the real-world crowd data. We propose a statistic model to calculate the similarity using Entropy Metric, and make use of MSI sources to deal with the large amount of computation.

Lead author: Ran Hu

MSI Principal Investigator: Stephen Guy (Computer Science and Engineering)

Title: A computational model of flow and species transport in the mesangium

Abstract: We constructed a computational model to understand accumulation of immune complexes within the kidney mesangium in IgA nephropathy. We calculate the influence of basement membrane thickness, mesangial matrix permeability, and immune complex size on accumulation.

Lead author: Sarah Hunt

MSI Principal Investigator: Victor Barocas (Biomedical Engineering; MSI Fellow)
Title: A stochastic framework for narrative generation with Monte Carlo Tree Search

Abstract: Planning-based techniques are powerful tools for automated narrative generation, however, as the planning domain grows in the number of possible actions traditional planning techniques suffer from a combinatorial explosion. In this work, we propose a Monte Carlo Tree Search based goal-driven narrative generator by using Multi-armed bandit techniques for exploration versus exploitation dilemma.

Lead author: Bilal Kartal

MSI Principal Investigator: Stephen Guy (Computer Science and Engineering)

Title: 1D nanodusty plasma sectional model with chemistry reaction for the study and control of particle generation and growth

Abstract: 1D nanodustry plasma model. Fabrication and control of nanoparticle size through chemistry interaction.

Lead author: Carlos Larriba-Andaluz

MSI Principal Investigator: Steven Girshick (Mechanical Engineering; MSI Fellow)
Title: Numerical simulation of 2D capacitively coupled RF plasma for the synthesis of silicon nanocrystals

Abstract: The poster will describe the set-up studied for the synthesis of silicon nanocrystals, along with preliminary results.

Lead author: Romain Le Picard

MSI Principal Investigator: Steven Girshick (Mechanical Engineering; MSI Fellow)

Title: Predictive screening of column pair combinations for two-dimensional liquid chromatography

Abstract: Two-dimensional liquid chromatography (2DLC) is a powerful separation technique that employs a second column to further separate fractions taken from the first column; when utilized in an on-line fashion, 2DLC can result in much higher total peak capacities than are achievable with a single column. This computational work addresses the significant challenge of selecting an optimal column pair from the N2 possible combinations (order matters in the on-line approach) by presenting a predictive screening method for column pair selection, and provides insight into the defining characteristics of a good column pair.

Lead author: Rebecca Lindsey

MSI Principal Investigator: J. Ilja Siepmann (Chemistry; MSI Fellow)
Title: Mining remote sensing data for land monitoring at a global scale

Abstract: We present spatio-temporal data mining research for monitoring land surface using terabytes of data collected by remote sensors. Our algorithms analyze terabytes of remotely sensed data to detect land change events such as fires, insect damage, and agricultural changes.

Lead author: Varun Mithal

MSI Principal Investigator: Vipin Kumar (Computer Science and Engineering; MSI Fellow)

Title: Bending of few-layer-thick boron nitride and graphene: Experiment and objective molecular dynamics calculations

Abstract: A localized kinking deformation is observed in few-layer boron-nitride and graphene nanoribbons under direct in-situ bending within a TEM. Objective atomistic simulations reveal the kinking to be due to a delamination of layers and provide quantitative predictions and morphological details in agreement with experiment.

Lead author: Ilia Nikoforov

MSI Principal Investigator: Traian Dumitrica (Mechanical Engineering)
Title: Distinct element approach for modeling carbon nanotube systems

Abstract: We present a distinct element concept for simulating morphologies and mechanical properties of carbon nanotube systems.

Lead author: Igor Ostanin

MSI Principal Investigator: Traian Dumitrica (Mechanical Engineering)

Title: Three-dimensional two-temperature modeling of plasma arc cutting

Abstract: In the present work, a 3-D numerical simulation using two-temperature model has been conducted for better understanding of plasma arc cutting.

Lead author: Hunkwan Park

MSI Principal Investigator: Terrence Simon (Mechanical Engineering)
Title: Multi-scale mechanical modeling of the Pacinian Corpuscle

Abstract: The Pacinian Corpuscle is a tactile mechanoreceptor that is located in the dermis of the skin and responds to high frequency vibrations within a large receptive field. A multi-scale finite-element model was used to determine the effect of geometry and receptor location on the response of the Pacinian Corpuscle to 10-micron indentation on the surface of the skin.

Lead author: Julia Quindlen

MSI Principal Investigator: Victor Barocas (Biomedical Engineering; MSI Fellow)

Title: A novel method to visualize and characterize the nanoscale 3D ultrastructure of plant cell wall using Transmission Electron Microscopy (3D-n-TEM)

Abstract: The poster aims to describe our work on characterization of the nanoporous structure of pretreated lignocellulosic biomass through electron tomography using 3-D Transmission Electron Microscope and the determination of mechanical properties of pre-treated biomass.

Lead author: Sahana Ramanna

MSI Principal Investigator: Shri Ramaswamy (Bioproducts and Biosystems Engineering)
Title: Genetic algorithm method to reconstructing mass distributions of galaxy clusters

Abstract: The genetic algorithm method known as Grale, was used to reconstruction the mass distribution of galaxy clusters through gravitational lensing. The mass distribution of several galaxy clusters, known as the Hubble Space Telescope Frontier Fields, were created to examine the distribution of dark matter relative to light matter.

Lead author: Kevin Sebesta

MSI Principal Investigator: Liliya Williams (Minnesota Institute for Astrophysics)

Title: Air quality impacts of conventional and alternative transportation fuels

Abstract: Much effort is being spent to switch from conventional spark-ignition gasoline vehicles to alternative fuels with improved environmental performance. Transportation fuel analysis usually focuses on emissions of greenhouse gases (GHG), but other impact categories, especially non-GHG air pollution, can also be important. In contrast to the impacts of GHG emissions from transportation, impacts from non-GHG air pollutants are highly dependent on the spatial location of emissions release. However, the few studies to investigate air quality-related public health impacts have struggled to capture their inherent spatial dependence. This spatially detailed life cycle assessment of ten alternatives to gasoline finds that electric vehicles powered by clean electricity are best for improving air quality.

Lead author: Christopher Tessum

MSI Principal Investigator: Julian Marshall (Civil Engineering)
Title: Using high performance computing to examine the effects of thermal gradients in carbonate CCUS reservoirs

Abstract: CO₂ Capture Utilization and Storage (CCUS) has promising prospects for mitigating the destructive consequences of anthropogenic greenhouse gas emissions and associated global climate change. In this presentation, we will explore CCUS operations involving cool CO₂ injection into geothermally warm, saline carbonate reservoirs using massively parallel reactive transport simulations.

Lead author: Benjamin Tutolo

MSI Principal Investigator: Martin Saar (Earth Sciences)

Title: The competition between N₂ and O₂ adsorption on open iron sites of the metal organic framework, Fe-MOF-74: A computational study by electronic structure theory

Abstract: The ability of the metal-organic framework, Fe2(dobdc), to fractionate a mixture of O₂ and N₂ is studied using quantum mechanical methods. The extended structure of Fe₂ (dobdc) is studied using cluster models that help us determine a number of properties (such as ground spin states and binding strengths) of the Fe-N₂ and Fe-O₂ interacting systems.

Lead author: Pragya Verman

MSI Principal Investigator: Donald Truhlar (Chemistry; MSI Fellow)
Title: CFD, modeling, and optimization of a heat exchanger used in a liquid-piston compressor

Abstract: Presented are the Anisotropic characterization of a heat exchanger and its applications in CFD (Computational Fluid Dynamics) simulations of a liquid-piston compressor and in an optimization problem of finding the optimal heat exchanger shape.

Lead author: Chao Zhang

MSI Principal Investigator: Terrence Simon (Mechanical Engineering)