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Dalmia (NYU Abu Dhabi)

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Programming for Biologists
The Brooklyn Research Cluster provides flexible computing, including for NYU Tandon's Visualization, Imaging, and Data Analytics research center.
• An app that translates sign language into spoken English using Brookyn Research Cluster Platform

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• Drug design for treatment of heart attack and stroke - How the hSCA N-1 enzyme is activated

• How carcinogenic chemicals slip past DNA repair mechanisms
NYU's Brooklyn Research Cluster provides a new way to network

Claudio Silva, who is professor of computer science and engineering and data science as well as co-director of Tandon's Visualization, Imaging and Data Analytics (VIDA) research center, and collaborators from the HPC group, NYU's central IT, and NYU Tandon are “so pleased to have launched a new resource that the entire university is benefiting from.” “VIDA is naturally making great use of the cluster but so are researchers from throughout Tandon, as well as from other NYU schools.” While officially still in alpha mode due to its deviation from the beaten path of traditional high-performance computing, the OpenStack-based Brooklyn Research Cluster is already being widely used by members of the NYU community, including many working in such areas as machine learning, web crawling, data analytics, and in complex applications like genomics browsers and sign-language translation.

An app that translates sign language into spoken English using Brooklyn Research Cluster Platform

A team of students from the NYU Tandon School of Engineering built the prototype of a mobile app that enables hearing people to understand sign language and helps the deaf by translating spoken words into sign language. Their project is part of the Verizon's Connected Futures challenge which, in partnership with NYC Media Lab, supports new media and technology projects from universities across New York City.

Zhongheng Li and his team used Brooklyn Research Cluster as their high-performance cloud computing platform to host their deep learning API using both OpenPose and TensorFlow trained Image classification model on the cloud. Initially, they wanted to use 'Depth Mode' camera features for better recognition. But, soon they realized that not everyone can afford a high-end smartphone model with depth camera features. So, they converted RGB images into skeleton images using OpenPose library for better accuracy and eliminated the need for a depth camera. They leveraged the power and flexibility of cloud computing to enhance their recognition model. Since they are using RGB camera and processing the information in the cloud, they don't have to depend on any devices or platforms. They can implement their framework on other technologies such as Hololens.
Drug Design for treatment of heart attack and stroke - How the hSCAN-1 enzyme is activated

Recently it was discovered that saliva of certain blood-sucking insects contains an enzyme which indirectly prevents the blood from clotting, and that humans have a homologous protein, named hSCAN-1. Drs. David Rooklin and Yingkai Zhang from NYU's Department of Chemistry, with Dr. Min Lu from UMDNJ, set out to find how it might be modified for use in heart attack and stroke treatments. The key lay in developing an understanding of how the protein is activated, and the group ran hundreds of molecular simulations at quantum mechanical and atomistic scales. With any one simulation using up to 64 processors and running sometimes for weeks, the group used NYU's HPC resources to complete the workload. From the results the trio elucidated the detailed enzymatic mechanism of the human protein. (more)

How carcinogenic chemicals slip past DNA repair mechanisms

In DNA, a guanine (G) base usually pairs with a cytosine (C) base, as in the first image. If the G base is damaged by a benzo[a]pyrene-derived lesion the nucleotide excision repair machinery catches, removes and replaces the damaged base pair. But experimental work by Professor Nicholas E. Geacintov of NYU Chemistry found that if the G base mis-pairs with adenine (A), the repair fails, leaving the DNA susceptible to cancer-causing mutation. Collaborating with Professor Geacintov and his team of experimentalists, computational researchers at NYU's Broyde Laboratory ran long-timeframe molecular dynamics simulations with AMBER on the NYU HPC facilities and found that the mis-pairing locally stabilizes the damaged DNA, hiding the damage from the nucleotide excision repair machinery. The image above indicates how a lesion would normally destabilize the DNA duplex, but with the incorrect partner (A) the destabilization does not occur. For more of the story and to see this much more vividly with visualizations from Professor Broyde's simulations, read on...

In this work many simulations of around 12,000 atoms each were run over 400 ns of simulated time. The Broyde laboratory is currently investigating nucleotide excision repair at the next higher order of DNA packaging, increasing the system size to a very computationally challenging 150,000 atoms.

An Event-Driven Model for Estimation of Phase-Amplitude Coupling at Time Scales of Cognitive Phenomena

Signal processing in neural science includes a wide variety of algorithms and methods of applied measurement that can produce very powerful correlations between the brain's computational ensemble of signals and the neurophysiological mechanisms that generate these signals. The sheer complexity and volume of the brain's electrical and chemical computational environment makes accurate detection of distinct brain wave oscillations a very difficult task for neuroscientists looking to justify analytical correlations of this traffic to any of the brain's computational mechanisms.

Recently, at NYU's Center for Neural Science, Dr. Andre Fenton and Ph.D student Dino Dvorak developed a new approach to phase-amplitude coupling (PAC) estimation between distinct neural oscillations which treats each oscillation as a discrete event rather than continuous time series of phase and amplitude. The approach proposes "oscillation-triggered coupling" (OTC) as a unified framework for PAC estimation that provides a
parameter-free, data-driven analysis for time windows that are considerably smaller than current, standard PAC estimation methods. This new framework provides the same information about PAC estimates as current methods (which require analysis windows of at least 10 seconds) while providing new insight toward proper PAC estimates at time scales which are on the order of a single modulation signal cycle. (read more)

This diagram shows the schematic decomposition of the global-scale analytical windows used for standard PAC estimation and the local-scale, OTC analysis detailed by Dr. Fenton and Ph.D student Dino Dvorak. The following graphs show the analytical process for interpreting the raw signals and generating PAC estimates within the OTC framework.

**Seeing below the resolution of MRI**

Biological tissue, porous rock and composite material samples appear uniform at the macro-scale and well-organized at the micro-scale, but their structural disorder at the meso-scale - such as the cellular level - is an important indicator for categorizing samples and identifying diseases.

One non-invasive technique is to measure molecular diffusion of, for example, water, through the sample. Mesoscopic structural parameters such as pore or cell sizes and shapes can then be inferred from the time-dependent diffusion behavior.

Making this inference is, however, a difficult and ill-posed problem, requiring a structural model which predicts the bulk diffusion coefficient, against which the measured one could be compared.

Drs. Dmitry Novikov and Els Fieremans of NYU School of Medicine, working with Drs. Jens Jensen and Joseph Helpern of the Medical University of South Carolina, have proposed that the structural disorder in a sample can be adequately and parsimoniously represented with just a small set of "structural universality classes", as illustrated below. These are characterized by a structural exponent $\rho$ in the relation $=(\rho+d)/2$, where $d$ is the number of spatial dimensions and is the dynamical exponent characterizing diffusion in the long-time limit. Dr. Novikov and colleagues used the NYU HPC clusters to run simulations, based on Monte-Carlo methods, showing the time dependent diffusion behavior of each structural universality class. (keep reading...)

Drs. Novikov and Fieremans's work is published in PNAS at [http://www.pnas.org/content/111/14/5088](http://www.pnas.org/content/111/14/5088).