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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 an 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)*

This diagram shows a previously uncharacterized catalytic calcium-binding site, shedding light on the sigmoidal relationship between enzymatic rate and calcium concentration.

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 NYUs 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.

The link between Atlantic Ocean warming and Antarctic climate change
In recent decades Antarctica, especially the Antarctic Peninsula, has experienced dramatic climate change, one observed phenomenon being a dipolar pattern of high sea-level pressure south of Australia and low sea-level pressure in the Amundsen Sea during the southern winter. The mechanism driving this has been identified by researchers at NYU's Center for Atmospheric and Ocean Science as warming in the north and tropical Atlantic.

Xichen Li, David Holland, Edwin Gerber and Changhyun Yoo recently published a paper in Nature showing that this pattern of Antarctic sea-level pressure correlates with sea surface temperature in the north and tropical Atlantic, moreover that the Atlantic sea surface temperature is driving the Antarctic sea-level pressure and that the low pressure thus established in the Amundsen Sea enhances warm-air advection and warm-water transport to the Antarctic Peninsula, thus contributing to the observed climate change in that region.

Xichen Li and colleagues used regression and maximum covariance analysis to establish the correlation between sea surface temperature in the north and tropical Atlantic, as illustrated below. However correlation does not imply causation, and physical experiments testing the effect on Antarctica of altering temperatures in the Atlantic are not practical (or ethical!). But by running numerical simulations on NYU's HPC clusters, using the Community Atmosphere Model (CAM4) from NCAR they were able to show that by forcing warming in the north and tropical Atlantic causes sea-level patterns in Antarctica corresponding to those observed. (read more)

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 $p$ in the relation $d/(p+d)/2$, where $d$ is the number of spatial dimensions and $p$ 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.
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.