ORACLES and PREDICTIONS

From weather forecasts to diagnostics…

Greek mythology tells of Cassandra, on whom the god Apollo had bestowed the gift of **prescience** together with the curse of never being believed. In our case, bypassing the gods, elegant **science** underlies the development of robust systems which predict weather, disease, molecular conformations and even musical tastes. This issue showcases technologies emanating from research in the departments of Atmospheric and Ocean Sciences (A&OS), Psychology and Chemistry.

How accurately can we predict the weather?

It is in the 1940's that radar (**ra**dio **d**etection **a**nd **r**anging) meteorology was born. Initially developed to track enemy planes, reflectivity data obtained from snow, hail or rain was tamed by McGill's J.S. Marshall so as to directly calculate the amount of impending precipitation. His equation is still used world-wide today.

Unique in Canada with its 10-cm pulse wavelength, the McGill radar can "see" beyond the current precipitation and predict the next location of storms. Emitting up to 1200 pulses per second and rotating at 6 rpm, it provides highly accurate forecasts of precipitation within three-to-five hours. In this time frame, precipitation prediction is much more accurate than model-based data and also supplies exact localization.

Networks of overlapping radar ranges, together with satellite data, allow composite views. Software tools have been developed to interpret the massive amount of data. The RAPID and MAPLE software developed by Prof. **Isztar Zawadzki** (A&OS) and his team are widely used for weather "nowcasting" and have been licensed for commercial use.

An important use of radar is to enable assessment of the amount of precipitation over large basins for hydrological purposes. In an ongoing collaboration with the Montreal Urban Community, precipitation forecasts by the McGill radar station are used to give early warnings of excessive accumulation in wastewater treatment basins. This enables the MUC to divert flows and manage the contents of its sewage holding tanks so as to maintain optimal filtration performance and safeguard the local environment.

Can we predict extreme weather?

It is known that small weather systems such as thunderstorms affect global weather patterns. But even though precursor atmospheric disturbances may be identified several days prior to thunderstorms or tornadoes, predictions of such extreme events are often poor. Atmospheric dynamics above 4 km often have a crucial impact on the development of precipitation-producing surface-level weather systems. But given the scant amount of data normally collected for vast unpopulated regions (such as oceans), weather models mainly guess at the state of the atmosphere. Wrong guesses can result in major forecast errors. A team working with Prof. **John Gyakum** (A&OS) has developed an automated suite of computer programs (IMPROVE) based on satellite total column ozone data. Available uniformly around the globe, the use of satellite data in a numerical weather prediction model enables a more accurate representation of the state of the atmosphere above these regions. And hence believable predictions…

Call it radar for health

Were health practitioners able to foresee complications or identify disease at an early stage, more lives would be saved and considerable costs potentially avoided. Prof. **David Burns** (Chemistry) and coworkers have discovered that spectroscopic analysis of fluid human tissue (e.g. amniotic fluid or blood plasma) in the near infrared region permits swift and reliable molecular fingerprints characterizing several health indications.

This scientific platform underlies the development of diagnostic technology which allows predictive monitoring in applications ranging from fetal and

respiratory health, through neurodegenerative disease and in-vitro fertilization. **Molecular Biometrics**, a McGill spin-off company created in 2005, is currently preparing to launch the first clinical diagnostic tool based on this technology, for applications in reproductive health.

Complementing the scientific break-through, strong social and economic benefits can also ensue. Considering the rise in human longevity, for example, the need to hone our capacity for early, non-invasive and accurate detection of age-related neural degeneration is critical. Early diagnosis would enable both patients and their family to make informed and timely social, legal and medical decisions about treatment and care. Even a modest delay in institutionalization would mean substantial social and financial savings. Conversely, a testing procedure that could rule out Alzheimer's disease would eliminate the tremendous uncertainty and anxiety patients and their families otherwise face and would allow physicians to focus on the other, potentially reversible, causes of cognitive dysfunction.

Predicting protein conformation

Large molecules in solution are anything but static… and proteins in the cell can adopt innumerable conformations depending on polar groups and other components in the intracellular fluid environment. For the synthetic chemists whose quest it is to develop a therapeutic drug, knowledge of the binding modes of potential durgs to this flexible object yields a stunning advantage in the ability to design a successful molecule.

Prof. **Nicolas Moitessier** (Chemistry) and his team have developed a suite of programs (FITTED 2.2) which simulate *in silico* the docking of flexible ligands onto flexible proteins. This software relies on a genetic algorithm to model the flexibility of the two molecules and, uniquely, factors in the location of ubiquitous water molecules. Switching functions serve to retain or displace water molecules and to model the formation of potential covalent bonds between the drug and the protein side-chains.

An integral part of the drug discovery process is the virtual screening of libraries of compounds in order to identify the promising few out of the thousands of available compounds, and to prioritize them for biochemical assays. This virtual screening is critical to the execution of a rational selection process. At present, almost all the docking protocols used are based on a rigid receptor model and do not take into account the mobility of the ensemble of amino acids that constitute the binding site of the ligand. FITTED 2.2 improves the accuracy of existing molecule docking software programs and uses optimized protein models based on a pharmacophore-oriented docking method.

The notable increase in accuracy of prediction of the actual docking process has resulted in several non-exclusive licenses of the software to companies working in drug discovery.

So what music will they choose?

In a culture characterized by exuberant choice in broadcast musical offerings, this question can be of particular interest to advertisers and providers of musical content. Prof. **Daniel Levitin (**Psychology) and collaborators have developed an adaptive learning music recommendation system that automatically suggests songs to listeners based on knowledge of past preferences, song descriptions, and personal demographic information.

This technology has been licensed to a leading developer of specialized Internet applications and music recommendation tools. Incorporated into their flagship product musicBOT, this invention is now the engine for a commercial product launched by Canadian media giant Astral Media.

In conclusion, the predictive tools developed by Profs. Burns, Gyakum, Zawadzki, Levitin and Moitessier provide data that is not only believed but also successfully being used in the ongoing drive to enhance our societal well-being.

RIO's biannual newsletter highlights research in the Faculty of Science which has led to technology being transferred to partners outside the university and commercialized. Readers who wish to receive RIO's newsletter electronically should contact erica.besso@mcgill.ca or call 514-398-3897.