St. Francis Xavier University

Physics Colloquium

Wednesday, 7 April 2010, 3:00pm, PSC 3046

Jeremy Thorbahn

Electrostatics-based Stealth Delivery Vehicles for Antimicrobial Peptides

Gram-Negative bacteria such as E. Coli and Salmonella are well known as food-borne pathogens. Hence, the ability to eliminate these harmful agents is very important in the advancement of food preparation and preservation technologies. Cationic antimicrobial peptides (CAPs) are able to destroy Gram-Negative bacteria if the peptides have access to the bacterial surface. Protamine, a 31-amino acid protein and the CAP we study, has 20 positively-charged amino acids which give the peptide its antimicrobial function, but leave it vulnerable to the influence of charged food proteins, polysaccharides and lipids before it ever reaches a bacterial surface. Therefore, an effective means of delivering protamine to destroy bacteria within a food requires a vehicle to shield peptides until they reach their target. Using Monte Carlo simulation, we model this delivery vehicle and examine its ability to effectively deliver protamine to the surface of Gram-Negative bacteria. Simulation results will be presented.

Megan Cuthbertson

Local Order Parameters in a Liquid-Liquid Phase Transition of Water

Water is one of the most important and ubiquitous materials in science as well as in everyday life. Despite being so common, it remains mysterious in many ways. Experiments have demonstrated the existence of two distinct phases of solid amorphous (glassy) water: high density amorphous ice and low density amorphous ice. An unresolved question is whether or not this same phenomenon is seen in liquid water. That is, do two distinct phases of liquid water occur in the supercooled regime? Using molecular dynamics simulations of the ST2 model of water, we investigate the properties of high density and low density liquid water. In general, thermodynamic phases are distinguished by order parameters. In this case, we use the local density, related to the distance of the 5th nearest neighbour molecule, as an order parameter to differentiate the two phases of liquid water in our simulations. We then study these phases under a variety of temperature and density conditions and investigate the critical point of this phase transition.

Marielle Lespérance

Propagation Of Linear Surface Air Temperature Trends Into The Terrestrial Subsurface

Previous studies have examined air and ground temperature relationships working under the assumption that linear trends in surface air temperature should be equal to those measured at depth within the terrestrial subsurface. A purely conductive model of heat conduction is used to show that surface trends are attenuated as a function of depth within conductive media, therefore invalidating the above assumption. The model is forced with synthetic linear surface temperature trends as the time varying upper boundary condition; synthetic trends are either noise free or include additions of Gaussian noise at the annual time scale. It is shown that over a 1000-year period, the trend is linearly damped with depth in both the noise-free and noise-added cases. When 100-year intervals are considered, the linear damping of the trend at depth is lost. An error estimate for the corresponding underground trend variation is determined by performing a Monte Carlo simulation. Using ECHO-G general circulation model output as a more realistic simulated data set, the damped trend behaviour as a function of depth is observed, although it is not linear. The use of air and soil temperature data collected over 99 years in Armagh, Ireland and 29 years in Fargo, North Dakota also do not show subsurface temperature trends that are equal to the surface trend. Over time scales smaller than 100 years and when noise is taken into account, damping of the temperature trend at depth is no longer observed due to the impact of annual variability on the trend estimates. It is therefore possible to observe the same trends at depth and at the surface, but such observations are not an indication that the ground and surface trends are directly coupled.