**Physics and Physical Oceanography Seminar**

## Honours thesis presentations

**DATE: Friday, Mar 12, 2021**
**TIME: 1:00 pm**
**Place: Webex (link will be sent out)**

**Presenter**: Matthew Williams
**Title**: Finite Difference Simulation of Interacting Resonance and Pulse Waves in a Nonlinear Material
**Abstract**: The field of nonlinear acousto-elastic behaviour in materials such as rocks is an area of active research, applicable to phenomena such as earthquakes or material fatigue. This nonlinearity arises from the rock microstructure, notably through cracks, and appears in the form of a nonlinear relation between the stress and strain fields within the rock. I study how this nonlinearity manifests when the sample is in either a resonant or a non-resonant state. To do this, I numerically model a sample including a crack and broadcast a low frequency pump wave and a high frequency probe wave through the sample. I use a fourth order finite difference scheme to model the evolution of wave velocity, stress, and strain, then use a form of averaging to represent the cracked, heterogeneous model with an effective homogeneous model. Calculating the nonlinear interactions between the two waves allows me to compare the resonant and non-resonant behaviour. I demonstrate differences in the effective wave velocity, and in the travel time delays between effective velocities with and without a pump source.

**Presenter:** Erica Short
**Title:** A Langevin dynamics based model for simulating polyethylene glycol
**Abstract:** Living cells are full of biopolymers such as proteins and RNA. Their diffusion is not well understood, especially biopolymers that are highly flexible such as polyethylene glycol (PEG). Diffusion is one of the main transport mechanisms for biomolecules inside living cells and is important to understand. My project is to develop a simulation of a model for PEG. PEG is a long polymer molecule and the model will be based on Langevin dynamics. I compare these simulations with available experimental (NMR) data on PEG diffusion coefficients. First, in our simulations, we measure the radius of gyration and examine how it scales with the number of chain beads. We then calculate the mean square displacement and, from it, the diffusion coefficient, in simulations of a single polymer chain and of multiple chains.

**Presenter:** Joseline Aimee
**Title:** Extracting the real and imaginary parts of a Photoacoustic Infrared spectrum
**Abstract:** Vibrations among atoms in a solid material can be triggered by absorbing infrared light. The energy associated with different kinds of vibrations, such as bending or stretching, are influenced by the types of atoms and their arrangements. Photoacoustic Fourier Transform Infrared Spectroscopy (FTIR-PAS) is an experimental technique that allows us to assess what energies of infrared light a solid material can absorb. My thesis research focuses on implementing mathematical tools and methods on previously Photoacoustic spectra to manipulate the data in a new way. The goal is to extract the real and imaginary parts of various photoacoustic infrared spectra. Once extracted, we analyze the data to determine whether there are consistent differences (or similarities) between the two as we keep the sample the same, but change the photoacoustic detection parameters and determine which additional terms have to be considered to account for these differences or similarities. A component of the research process is to determine which programming tools and software are efficient to conduct the data manipulation. My talk will explain how we investigate whether differences between the real and imaginary parts of the FTIR-PAS spectrum are related solely to instrumentation effects, or if they can tell us useful information about the structure about our solid samples.

ALL ARE WELCOME!