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PH235 Final Project Proposal

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Describe your project, project members, roles and each member’s contribution should be clearly specified for teams.

The aim of this project is to simulate the behavior of gas phase chemical reaction systems. In particular, bimolecular reactions of the form A + B C + D will be considered. The user will first enter the two starting reactants A and B. The program will then search a previously prepared file that contains a list of possible bimolecular reactions and parameters to be substituted into the Arrhenius rate equation given below:

**k(T) = A (T/298 K)n e-Ea/RT**

The parameters A, n and Ea will be obtained from the NIST database: <http://kinetics.nist.gov/kinetics/index.jsp> by writing a web scraping program.

The Arrhenius equation allows for the calculation of the rate of a reaction at a given temperature, which will also be entered by the user. The rate constant essentially tells us how quickly the reactants will be converted to products. If the reaction is reversible, there will also be another rate constant which describes the rate at which the products C and D convert back to A and B.

Using the Gillespie algorithm, the concentrations of reactants and products for a given temperature will be calculated and plotted over time. A summary of the Gillespie algorithm, omitting the math, is given below:

1. Initialization: Initialize the number of molecules in the system, reaction constants, and random number generators.
2. Monte Carlo step: Generate random numbers to determine the next reaction to occur as well as the time interval. The probability of a given reaction to be chosen is proportional to the number of substrate molecules.
3. Update: Increase the time step by the randomly generated time in Step 2. Update the molecule count based on the reaction that occurred.
4. Iterate: Go back to Step 2 unless the number of reactants is zero or the simulation time has been exceeded.

Enumerate the PH235 related topics (questions and solution approaches) each individual will contribute to the project.

This project will encompass the following Ph235 topics and solution approaches: random stochastic processes, the Gillespie Algorithm (a type of dynamic Monte Carlo method), optimizing code for computationally expensive simulations, solving differential equations, as well as graphical displays of species concentrations over time.

Describe what you plan to demo on the final exam date and other deliverables (project webpage is required).

On the final exam date I plan to demo the web scarping program for extracting data from the NIST database (the possible reactions that can occur depending on the reactants entered by the user and parameters that allow for the calculation of the rate constant at the temperature entered by user) and several time varying plots constructed from Gillespie algorithm calculations.

Describe your plan to evaluate the project.

I plan to evaluate the calculated species concentrations by comparing them to the concentrations calculated by solving the differential rate equations. I will solve the equations for a few selected reaction systems using one of the methods we have learned in class and plot the concentrations calculated using the Gillespie algorithm on the same graph as those calculated by solving the differential equations. This comparison / evaluation will be the last part of the in-class demonstration.

Identify expected low hanging fruit, challenges and contingency plans where possible.

Modifications to the Gillepsie algorithm may have to be made in order to reduce the run time of the simulation. The Gillespie algorithm is very computationally expensive and many modifications and adaptations exist, including the next reaction method (Gibson & Bruck), [tau-leaping](https://en.wikipedia.org/wiki/Tau-leaping), as well as hybrid techniques where abundant reactants are modeled with deterministic behavior. One or more of these modifications may be used. In addition, some bimolecular reactions may be omitted because they give rise to too many intermediate products even though the stable state system may only contain two products.

Provide a schedule/timeline for your progress for November and December including following mandatory key dates:

I will first create a simple program that uses the Gillespie algorithm to calculate the species concentrations of a simple bimolecular reaction. This will allow me to refine parameters such as initial concentrations of reactants in order to optimize run time and accuracy.

Then I will write a web scraper program that extracts the kinetics data from the NIST website.

Finally I will incorporate the data obtained from NIST with the Gillespie algorithm to create an interactive program that allows the user to predict the behavior of two reactants at a certain temperature of their choice.