Fortran & MD

Learning Outcomes

- Students will be able to describe how molecules and atoms move based on kinetic molecular theory.
- Students will be able identify the factors that affect molecular motion
- Students will be able to give examples of how computer simulation is used in chemistry.
- Students will be able to summarize the process by which a computer calculates molecular motion and structures.
- Students will be able to analyze the results of the simulation to compare them to their hypotheses.
- Students will be able to graph and analyze data such as energy and temperature variations) from the simulation
- Students will be able to modify a computer simulation and compare the resulting data to the original simulation.

MA State Standards Addressed

- 9-12.DTC.a.1 Use digital tools to design and develop a significant digital artifact (e.g., multipage website, online portfolio, simulation).
- 9-12.DTC.b.1 Communicate and publish key ideas and details to a variety of audiences using digital tools and media-rich resources.
- 9-12.CT.c.6 Analyze a complex data set to answer a question or test a hypothesis (e.g., analyze a large set of weather or financial data to predict future patterns), individually and collaboratively.
- 9-12.CT.e.1 Create models and simulations to help formulate, test, and refine hypotheses, individually and collaboratively.
- 9-12.CT.e.2 Form a model from a hypothesis generated from research and run a simulation to collect and analyze data to test that hypothesis, individually and collaboratively.
- 9-12.CT.d.1 Use a development process in creating a computational artifact, individually and collaboratively, that leads to a minimum viable product followed by reflection, analysis, and iteration (e.g., data-set analysis program for science and engineering fair, capstone project that includes a program, term research project based on program data).
- 9-12.CT.d.2 Decompose a problem by defining functions which accept parameters and produce return values, individually and collaboratively.
- 9-12.CT.d.3 Select the appropriate data structure to represent information for a given problem (e.g., records, arrays, lists), individually and collaboratively.

- 9-12.CT.d.5 Use appropriate looping structures in programs (e.g., FOR, WHILE, RECURSION).
- 9-12.CT.d.6 Use appropriate conditional structures in programs (e.g., IF-THEN, IF-THEN-ELSE, SWITCH).
- 9-12.CT.d.8 Use a programming language or tool feature correctly to enforce operator precedence. Use global and local scope appropriately in program design (e.g., for variables).
- 9-12.CT.d.9 Select and employ an appropriate component or library to facilitate programming solutions (e.g., turtle, Global Positioning System (GPS) component, statistics library, Scratch).