The objective of this research was to determine if a better understanding of the "molecule of life", deoxyribonucleic acid or DNA can be obtained through Molecular Dynamics (MD) modeling and simulation (M&S) using contemporary MD M&S. It is difficult to overstate the significance of the DNA molecule. In addition to the fact that DNA contains the informational blueprints for all life, it also exhibits other remarkable characteristics most of which are either poorly understood or remain complete mysteries.

One of those completely mysterious characteristics is the ability of DNA molecules to spontaneously segregate with other DNA molecules of similar sequence. This ability has been observed for years in living organisms and is known as "homologous pairing." It is completely reproducible in a laboratory and defies explanation. What is the underlying mechanism that facilitates long-range attraction between 2 double-helix DNA molecules containing similar nucleotide sequences? The fact that we cannot answer this question indicates we are missing a fundamental piece of information concerning the DNA bio-molecule. The research proposed herein investigated using the Nano-scale Molecular Dynamics NAMD simulator the following hypotheses:

- **H(Simulate Observed Closure NULL)**: Current MD force fields can reproduce directed segregating movement (closure of homologous segments).
- **H(Resonance NULL)**: Current MD force fields can reproduce theorized molecular resonation in the form of frequency content found in water pressures between the segments.
- **H(Harmonized Resonance NULL)**: Current MD force field models of DNA molecule segments can reproduce frequency content above and beyond the expected normal frequency levels found in water.
- **H(Sequence Relationship NULL)**: The specific frequencies and amplitudes of the harmonized resonance postulated in H(Harmonized Resonance NULL) are a direct function of DNA nucleotide sequence.
- **H(Resonance Causes Closure NULL)**: Interacting harmonized resonation produces an aggregate force between 2 homologous DNA segments reproducing closure.

No evidence of closure between two similar sequenced DNA segments was found. Fourier analysis of pressures revealed a rich selection of periodic pressure variation occurring in the solvent between simulated DNA molecules. The pressure data was characterized as statistically significant and was located in less than 2% of the coefficients by count. This unexpected result occurred consistently in 5 different system configurations with considerable system-to-system variation in both frequency and magnitude. Given the extent of the experiments the data was found to be in support of H(Resonance NULL), and H(Harmonized Resonance NULL). Regarding the emergent hypothesis H(Sequence Relationship NULL), conflicting results were inconclusive so the hypothesis was neither accepted nor rejected. Of particular interest to future researchers it was noted that the computational simulations performed herein were NOT able to reproduce what we know actually happens in a laboratory environment. DNA segregation known to occur in-vitro did not occur in our simulation.

Major: IDS Modeling and Simulation

Educational Career:
Bachelor's of BS Engineering - EE, BS, 1987, UCF

Committee in Charge:
Michael D. Proctor, Chair, IEMS
J. Peter Kincaid, IST
Jaganathan Bala, IST
Karl X. Chai, College of Medicine
Matthew Gerber, College of Medicine

Approved for distribution by Michael D. Proctor, Committee Chair, on July 22, 2011.

The public is welcome to attend.