2009 Women in the Sciences and Engineering (WISE) workshop



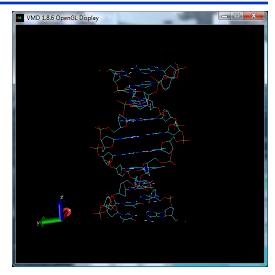
"Building, Simulating and Analyzing Polymers Using Computational Chemistry"



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A total of 48 women between the ages of 15 and 17 participated in a weeklong science and engineering summer camp at Penn State's University Park campus. In this workshop the group was introduced to computational chemistry and the molecular modeling technique of molecular dynamics (MD). One of the main goals of this workshop was to introduce the students to a field which they had most likely never been exposed to.

Each participant connected to one of Penn State's powerful computing clusters and ran their own molecular dynamics simulation of a short segment of DNA using software program AMBER. The students were then able to "watch" the progression of the simulation with the visualization program VMD.



Simulation snapshot: DNA fragment





