Cornell CS 322 - Intro to Scientific Computing

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Applications of Numberical Methods for Molecular Modeling

Tuesday, March 4th, 2008 3:40 am
Written by: **somestudent**

Several of the previous posters already addressed the applications of numerical computation to modeling molecules and atoms. While searching for an article for this post, I found an interesting example of such research here. The study, by Bern Kohler and Yu Kay Law, looks at DNA damage from UV rays.

A DNA molecule can take on billions of different positions and shapes. The researchers modeled what occurs to a DNA molecule in different positions when it in is hit by a ray of UV light coming from different directions s. They found that DNA molecules cannot be damaged by UV rays in most positions. However, if the molecule is "in the wrong place at the wrong time" it can sustain damage that can lead to skin cancer. These findings explain why skin cell DNA damage occurs on some place on the molecule much more often then others.

Because of the number of possible shapes the research was carried out at the Ohio Supercomputer Center.

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