VISAR — Visual Interactive Structural Analysis Reporter

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VISAR is a visual graphics tool created for the purpose of facilitating analysis of structural molecular data that is generated by an optimization program.

Typically, an optimization program runs on a supercomputer. The results of the calculations are numeric, and interpretation of the data obtained is very difficult due to the vast data amounts.

VISAR lets users see the result of a calculational step as a frame in a "movie." It displays the molecule structure resulting from each step in perspective. VISAR then proceeds to show all calculational steps, thereby creating a "movie" that cuts result analysis time greatly, as well as giving the viewer a clear feel for where particular atomic interactions are taking significant effects.

Along with each frame, VISAR displays a window of information pertinent to the frame, such as the total potential energy of the system.

Interaction with the user takes place via a mouse and pop-up menus. The viewer can stop VISAR at any frame of interest. The interesting molecule's data can then be stored into a file for further analysis, if necessary. In addition, VISAR allows each frame to be rotated in three dimensions so as to allow better visual access to initially hidden parts.

VISAR allows the viewer to jump back and forth to any desired frame in the movie, and also allows a feature of gentle rocking motions for each frame in any direction, so as to give a better three-dimensional (3D) feel.

VISAR also has a stereo mode. Using green-red stereo separation coupled with the appropriate polarized eyeglasses, it is possible to get quite a realistic 3D view at a very low cost (the cost of the glasses).

Further features now being applied to VISAR include the facility for the viewer to point to any pair of atoms and see certain desired parameters about their interactions being displayed, even as the molecule is in motion. These parameters will change values in accordance with the state of the molecule in each frame (e.g., if the parameter is the electrostatic force between two atoms, it will be displayed continuously, with the figure changing to reflect the actual force as it varies from frame to frame). In addition, various statistics are gathered and will be displayed in separate windows.

VISAR was created on a Silicon Graphics IRIS model 3030 graphics workstation, and it makes extensive use of the windowing environment available on that machine.

Modeling Nucleic Acid Hydration

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Recent improvements in crystallographic data for oligonucleotides have enabled reliable identification of many individual solvent molecules. Ordered patterns of hydration have been observed and constitute an important element in stabilizing specific sequences and specific secondary structures of DNA.

A simple approach to understanding solvent structure around a macromolecule is the hydration site method, which determines the primary local minima of the interaction energy of one solvent molecule with the whole macromolecule. This method ignores the cooperative effects between hydrogen-bonded water molcules, but does not require such large computer power as computer simulation techniques. Qualitative and quantitative information about the possibility of hydration of the polar and ionic groups of the molecule can be obtained very rapidly.

In order to get insight into the influence of interactions of water with oligonucleotide conformations, we used this approach to initiate a systematic survey of solvation of the phosphate backbones, the bases, the minor and the major grooves for DNA in the different helical forms.

In a first step, we tried to quantify the effect of sequence variations on the hydration of the classical averaged helical forms (A, B, Z). The A form favors the formation of bridging sites on the phosphate groups and on the bases. For B structures, the water bridges connect atoms of the bases, while the phosphate groups are individually hydrated. Conversely, for the Z forms, water molecules bridges adjacent phosphate groups and phosphate groups to the bases, which can be also individually hydrated. These results are consistent with the concept of economy of hydration; however, other factors, such as entropic effects, may be important in stabilizing specific sequences.

In a second part we studied the effect of local variation in structure by comparing hydration sites for oligonucleotides in crystal forms and classical helical forms. It appears that these local variations of structure are associated with rather large differences in the hydration potentiality, favoring the formation of ordered structures. More specifically, we showed that the B dodecamer d(CGCGAATTCGCG) adopts in the crystal a conformation with a narrow minor groove in which all its hydrogen bond possibilities with water are satisfied, leading to the formation of the famous spine of hydration.

Rendering Volumetric Data in Molecular Systems

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A ray-tracing method of rendering sampled scalar functions has been layered over RMS,[1] an existing z-buffer-based program for the representation of molecular van der Waals surfaces. Calculation of a raster image is performed directly from three-dimensional volume data,