

'*exploratory programming*⁴ so that the rules and prediction heuristics can be developed on an experimental basis, in close association with the 3D modelling. The system is based on our networked numeric, symbolic and graphic facility, using VAXen, E&S and Silicon Graphics displays, and Symbolics Lisp machines running KEE (Knowledge Engineering Environment). Input is in the form of sequence list(s), assignments of secondary structure, and assignment of β -strands in any sheets. These may be generated by any one, or combination of predictive schemes, or for calibration purposes, the assignments given by experimental data from known proteins. At present the display rules use idealized helix and β -strands with idealized orientations of β -strands to form sheets, and orientations of helices to sheets. Preliminary work has been done on the RecA protein⁵. Further work is in progress to elaborate on the rules, and to extend the possible restrictions on turn geometries.

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The UCSF computer graphics laboratory: tenth anniversary progress report

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In 1970 the Division of Research Resources of NIH established the Computer Graphics Laboratory at Princeton University as a National Research Resource with the first E&S display, the LDS-1, hosted by a DEC PDP-10. Extensive software for protein and nucleic acid manipulation, analysis and stereo display was developed¹. In 1976 NIH transferred support to UCSF and we installed the first E&S PS2 interfaced to a DEC PDP-11/70 and wrote the first Unix-based 3D graphics package for the PS2 in the C programming language². By mid-1978 software was in place for selective black-and-white stereo display of both skeletal models and the Richards solvent accessible surface. The addition of real-time colour for the PS2 in late 1979 made the study of interactions much more comprehensible, particularly with dot representations of the Richards surface³. In 1981 we redesigned and integrated the software into

Midas (Molecular interactive display and simulation). New features were added, including electrostatic⁴ and real-time van der Waals surfaces⁵. Since 1977 over 100 investigators from 15 states and 10 countries have worked at the Laboratory, producing over 200 related publications. We have also converted Midas to other operating systems and displays, and it is now in use in over two dozen installations around the world. In 1983 we began the integration of 3D interactive graphics (based on Midas), with both numeric and symbolic computing now using KEE (the Knowledge Engineering Environment). Software is now running on a variety of machines, including VAXen, SGI and E&S 3D displays and Lisp machines, which communicate at up to 10 Mbit/s over an Ethernet. Prototype applications include protein engineering (Proem: protein experimental modeller)⁶ and drug design (Karma: Kee assisted receptor mapping analysis)⁷. Future plans for the Laboratory will be outlined.

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Exploring the unfolding of proteins

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Jane Richardson's ribbon representation of protein structure is greatly admired. Using bold aesthetics she has simplified protein structure to the point where we can begin to understand the architectural themes in the evolution of proteins. Because the ribbon diagrams take considerable time and skill to produce, several people, notably Arthur Lesk, have written programs to automatically make roughly equivalent representations. For many years I have wanted to think of proteins as space curves but I could not find a suitable representation. Several weeks ago I and my coworker Bernard Brooks developed a fitting procedure using GEMM (generate, emulate, and manipulate macromolecules). The atoms