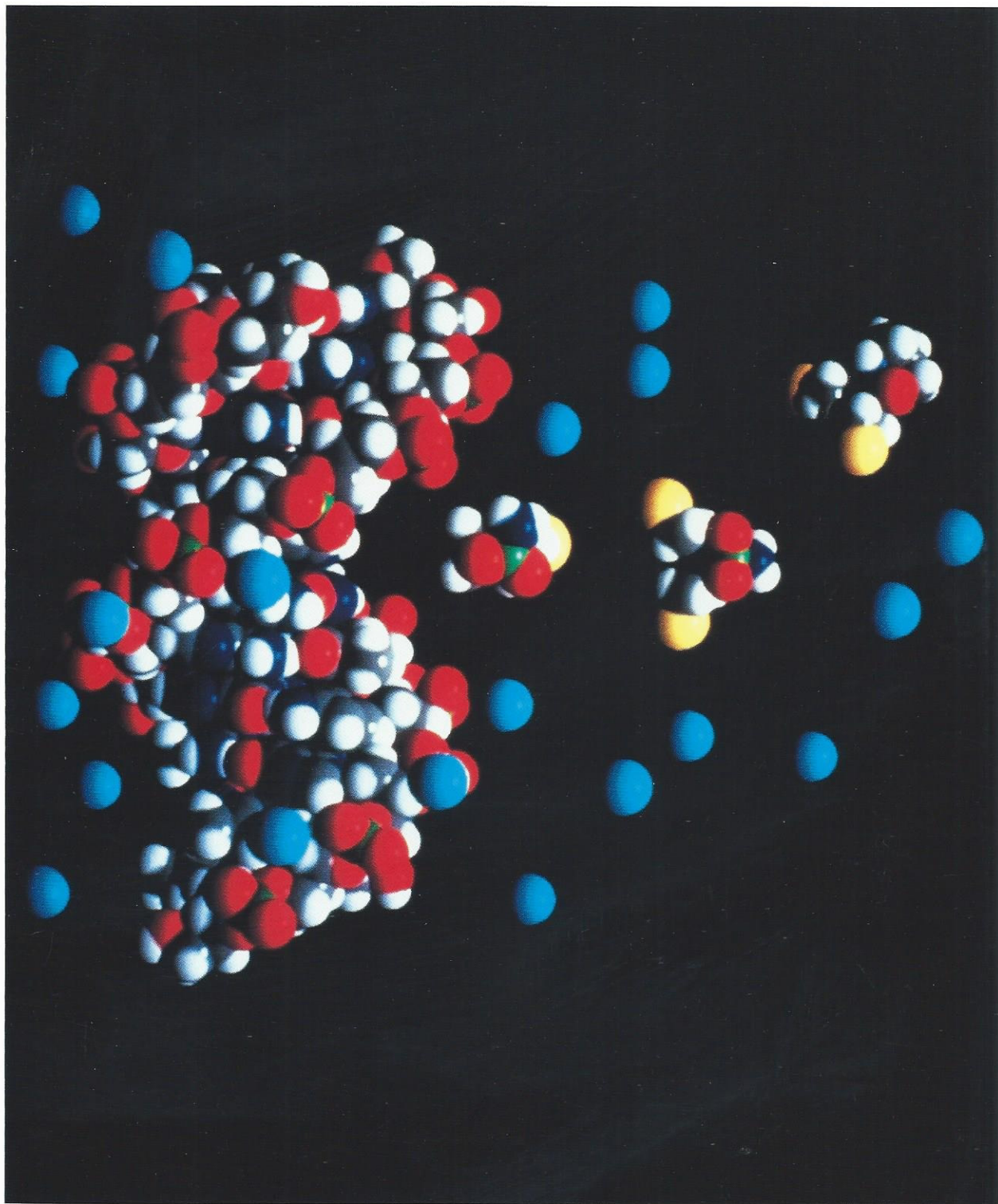


Applications Software for Cray Supercomputers



July 1988

CRAY

Applications Software Available for Cray Supercomputers

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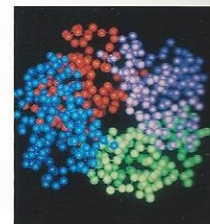
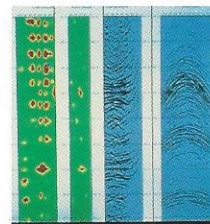
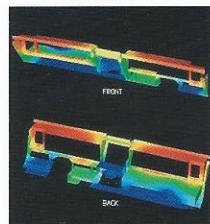
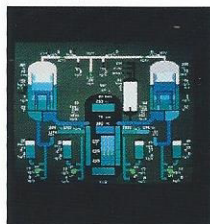
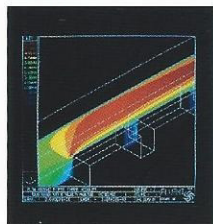
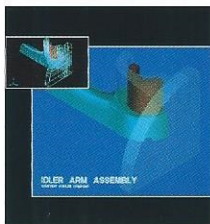
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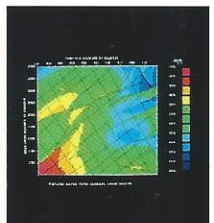
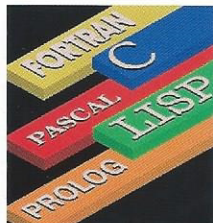
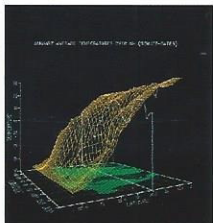
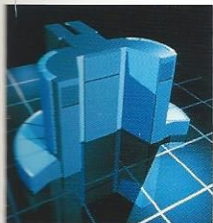
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Cray simulation of interrelated biomolecular pharmacology. On the left is an energy refined DNA structure surrounded by sodium counterions (light blue) which has been recently identified in human cancer cells. The structures shown at the right are cyclophosphamide and two reactive metabolites of this anticancer agent believed to have a major role in killing cancer cells by DNA interaction. The DNA molecule was energy minimized with the molecular mechanics/dynamics program AMBER, and ab initio calculations of cyclophosphamide and metabolites were done with the program GAUSSIAN-82 by Dr. Fred Hausheer (Johns Hopkins Pharmacology/Medical Oncology/National Cancer Institute).