PROGRESS AND PROSPECTS IN EXTREME SCALE SUPERCOMPUTING IN BIOLOGY, BIOENERGY AND MEDICINE

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The ramping up of the National Leadership Computing Facility at ORNL brings new opportunities for advances in biology, bioenergy and drug discovery. Examples will be given of scaling and applications in multimillion-atom molecular dynamics simulation of cellulosic ethanol systems in the framework of the DOE Bioenergy Science Center, and in the virtual docking of millions of compounds to potential drug targets. We describe strategies for optimal utilization of exascale supercomputing in biomolecular research, and describe the types of problems that might then be within reach.