

## Topological Bio-molecular Steering

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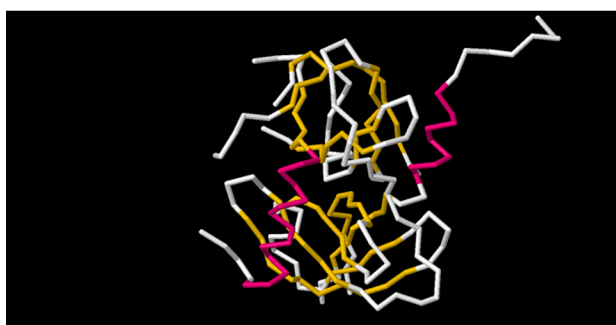
University of Connecticut

Digital Media Center

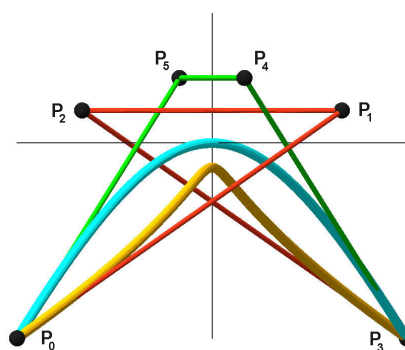
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(a)



(b)

Computational steering and dynamic visualization are seen as central for scientific discovery from the peta-byte output of bio-molecular simulations on Blue Gene/P. Informal analyses do not scale well and can mislead scientists. Topology is now providing appropriate formal foundations. Recent investigations on the protein data base will be shown, with experimental software and computational theorems. When the topological abstractions are complemented with aesthetic considerations, scientific discovery is further enhanced – a transdisciplinary approach pervasive within the recently established Digital Media Center at UConn. The talk will conclude with speculative remarks about the role of visualization and high performance computing in the emerging Jackson Laboratories Research Facility in Connecticut.

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