THE UNIVERSITY OF TENNESSEE
CHATTANOOGA

DEPARTMENT OF MATHEMATICS AND SIMCENTER

present

"A study of entanglement in physical systems and its relation to material properties and function"

by

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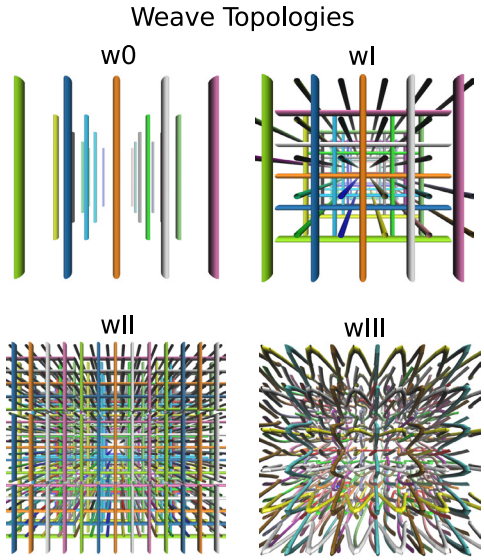
September 28th, 3 p.m., UTC SimCenter Auditorium*

Networking | Light Refreshments | Seminar | Q & A

Public Invited

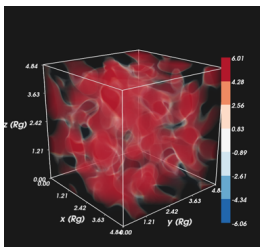
Many physical systems, such as biopolymers and polymer melts, are composed by macromolecules which cannot cross each other and attain entangled conformations. The entanglement complexity in these systems affects dramatically their mechanical properties. In this talk we will see methods by which one can measure entanglement in collections of open or closed curves in 3-space and in systems employing Periodic Boundary Conditions (PBC).

We show how our results can be used in practice by performing fully three-dimensional computational simulations of polymeric chains entangled in weaves of a few distinct topologies and with varying levels of chain densities. Our topological measures of entanglement indicate the global topology is the dominant factor in characterizing mechanical properties.



We also discuss the role of entanglement in proteins and how it correlates with protein folding kinetics. Our aim is to introduce a new model of protein folding kinetics that supports the prediction of a protein's folding rate from the topological and geometrical structure of its native state.

Finally, we discuss how polymer architecture can affect material properties. Using Field Theoretic Simulations we show how varying the number of arms in bottlebrush polymers leads to instantaneous nematic phase transition.



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