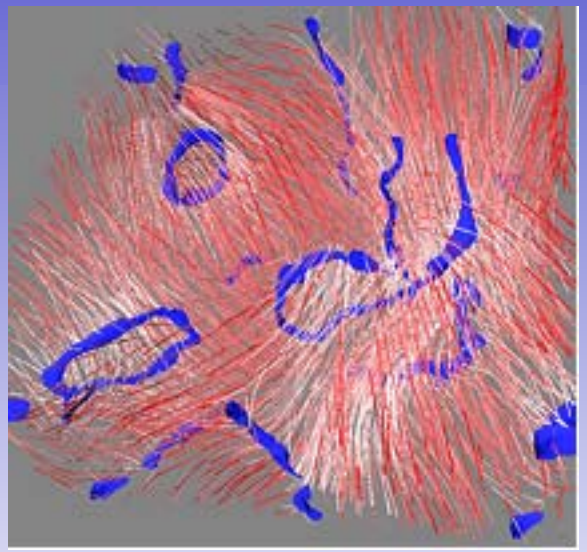
Visualization of Topological Defects in Liquid Crystals

Robert Pelcovits and George Loriot, Brown University, DMR 0131573

Trying to extract the key physical features of a complex system simulated on a computer is a challenging problem which can sometimes be solved using scientific visualization techniques. The ordering of liquid crystal molecules is described by a second-order tensor field, as is the anisotropic diffusion of water in biological tissues. Using techniques developed by our computer science collaborator, David Laidlaw of Brown, to visualize brain MRI scans, we have located topological defects in the liquid crystal ordering field and characterized the properties of these defects. The simulated system consists of 65536 molecules in a box. Direct imaging of the molecules would yield little direct information about the defects, but by visualizing the tensor field, defects can be immediately discerned.



Visualization of defects in the simulation box. The blue lines represent the defect loops. The red lines are “streamtubes” indicating the direction of local ordering of the rodlike liquid crystal molecules.

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Student involvement:

Vadim Slavin, CS graduate student
Andrew Callan-Jones, physics graduate student

Outreach:

Pelcovits organized a Group Research Project at Brown, involving undergraduates from CS and physics with this visualization project.

One of the major advantages that students in the field of scientific computation enjoy is their ability upon graduation to work in areas different from their thesis work, precisely because they have been trained in simulation techniques with broad applicability. Upon leaving our group our graduate students are well trained in the use of parallel computers and visualization techniques for modeling physical systems.