



YCCSA Seminar Series Autumn 2018

An interdisciplinary seminar series hosted by the York Cross-disciplinary Centre for Systems Analysis aimed at researchers from all disciplines

Surveying Energy Landscapes: From Protein Folding to Bistable Liquid Crystal Device and Cylindrical Buckling

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Friday, 14 December 2018

Ron Cooke Hub, RCH/204 at 13:30

Abstract:

Given a Hamiltonian or energy functional, I will describe a suite of numerical methods designed to efficiently characterise its energy landscape. The methods allow systematic study of not only the most relevant minimum energy configurations, but also the transition pathways between any two minima, as well as their corresponding energy barriers and transition state configurations. I will then illustrate the versatility of the methods by studying three very distinct problems. First, using a multistable liquid crystal square well as an example, I will provide insights into how optimal transition pathways can be qualitatively different even though the minimum energy configurations remain similar, and how certain minima can lose stability. Second, I will study how thin cylindrical shells buckle. In particular, I will discuss the large number of minima we observe and whether we have a glassy or a structure-seeker energy landscape. Third, while efficient algorithms for cluster detection and data completion in high-dimensional spaces are well developed, considerably less is known about the reliable inference of state transition dynamics in such settings. Here I will show how we can reconstruct low-dimensional dynamical transition networks from high-dimensional static samples, and demonstrate the practical potential of our scheme for several protein folding transitions.

The seminar includes a refreshment break to fuel interdisciplinary discussion

***Ron Cooke Hub is on Heslington East Campus – accessible by free bus services
Nos. 66 and UB1 running at frequent intervals from Heslington West.
The YCCSA Seminar room is on the second floor***