Telluride Workshop on The Complexity of Dynamics and Kinetics in Many Dimensions

August 13-24 2007
Camel's Garden Resort Hotel
Telluride Science Research Center (TSRC)
Telluride, CO, USA

Social Events

August 13: After the today's workshop
Bear Creek Hiking (2hours)
August 13: 18:00- Opening Reception (15US$ for each)
August 14: 18:00-19:15 Pinhead Town Talk
August 16: Photo After the morning session
August 16: 18:00- Picnic at the Garden in Telluride Lodge
August 21: 18:00-19:15 Pinhead Town Talk
"Nuclear Power and Climate Change: Choosing a Course Beyond Emotions"
Speaker: Professor R. Stephen Berry
August 23: 18:00-Picnic at the Garden in Telluride Lodge

Program

August 13: Setting an agenda of the topics to be discussed

Period of Stay

1st week: Aniruddha Chakraborty, Sergy Grebenshchikov, George Haller, Manuel Inarrea, Michael E. Kellman, Jesus Palacian, Ana I. Pascual, Vered Rom-Kedar, Vivian Tyng, Patricia Yanguas (10 people)

Both weeks: Thomas Bartsch, R. Stephen Berry, Johannes-Geert Hagmann, Jason Green, Charles Jaffe, Tamiki Komatsuzaki, Hiroshi Teramoto, Turgay Uzer, Holger Waalkens, Chengju Wang, Tomohiro Yanao, Laurent Wiesenfeld (15-), Mikito Toda (16-) (13 people)

General Agenda and Several Key Words

What is the underlying principle of complexity in kinetics and dynamics in many-degrees of freedom systems for a wide range of diverse systems such as three body systems, clusters, proteins and DNA?

Can we have common language, concepts and methodologies to cover through or bridge among complex systems of different space and time scales?

Key Concepts: Transition States (TS), Normally Hyperbolic Invariant Manifold (NHIM)?, Lagrangian Coherent Structure (LCS)? Nonlinear Time Series Analysis? Their Quantum Counterparts? Notion of potential and free energy Landscape, Billiard problem,...

Related with NHIM:

NHIM (stable against perturbation) and cylindrical invariant manifolds composed of its stable/unstable invariant manifolds can mediate chemical reactions even in a sea of chaos

1. Stability of NHIM in dissipative systems & Mechanism of Breakdown of NHIM: How NHIM can robustly survive under thermal fluctuation?

2. Quantum counterpart of classical NHIM: classical chaotic phase space and quantum “regular” structure

3. Local Ergodicity (Phase Space Geometry inside Potential Basins, NHIM inside Potential Basins): How NHIMs are `connected’ by the stable and unstable manifolds through the entire phase space ?

4. Some experimental evidence to support the versatility of the concept of NHIM? Ozone Chemistry, Some Chemical Reactions, or Hundreds/Thousands of Dimensions?

Related with NHIM:

Ambition to Multiscale Systems such as Proteins, DNA

1. NHIM in dissipative systems: How NHIM can robustly survive under thermal fluctuation?

2. I it possible to find a set of NHIMs for a space of, say, hundreds of dimensions? In addition, any possible means to address the geometrical structure of the state space? LCS? Finite Size Liapunov Exponent? Embedology? ...

3. Is there a useful way to find the NHIM of a complex system in terms of a drastically reduced set of variables, e.g. principal coordinates?

4. Can we utilize the concept of NHIM in multi-scale simulation as an efficient strategy for computations ?

5. Relevance to the implication of Robustness of Biological Functions?

Some other Interesting Topics

1. quantum dynamics is often governed by a particular symmetry. Is there a consistent way of constructing trajectory-based/TST-type methods taking symmetry (for example, spatial symmetry) into account?

2. Is there a consistent way of inclusion of zero-point energy effects in the TST description of chemical reactions?

3. Can a new paradigm for studying Hamiltonian systems with **steep potentials** be of use for studying chemical reactions? Can it be of use for identifying the relevant LCS/NHIM for these systems?

Complexity in Kinetics, Dynamics and Energy Landscapes in proteins and complex systems

1. What kinds of strange kinetics or dynamics are observed in real systems like clusters and proteins?

2. Is there any new dynamical concept or methodology to dig into the state space of large systems with multiscale time and space scales?

3. How can one quantify the complexity of energy landscapes such as multiple pathways in terms of characteristics of the topography of multidimensional landscape?

4. If there are multiple pathways between major minima, what is the significance--and the signature--of significant interconnectivity or independence of those pathways?

5. Can we find or invent new, summary variables that can describe the dynamics or kinetics of a system moving on a very high-dimensional landscape? analogous to the way thermodynamics allows us to work with a small set of variables?

- Is there geometric phase (out of the BO principle) associated to NHIM? See ozone as a trigger for the question, think in terms of Li_3 (RSB)
- - Advanced topics associated to NHIM:
- How can we treat multiscale systems such as proteins or DNA? Is it possible to find a set of NHIM for a space of hundreds of dimensions? How can we analyze the structure of the geometric space? Is there a useful way to find the NHIM of a complex system in reduced coordinates, eg. PC? Implication of robustness for biological systems? How to incorporate noisy dynamics into analysis of phase space? (TK)
- - In a complex systems, can internal modes, through mode coupling, act as a heat bath for the reaction? (RSB)- Comment: From experiments of small molecules, it is clear that what you learn from the gas phase remains valid (on a certain timescale) for the solute case. However, if you put the molecule on a surface, the situation is very different.
- -> question of robustness with respect to the environment (MK, TK) special case of non-perturbation of the environment that could be an extension of NHIM to the quantum case: superfluid helium clusters (RSB)- Is it possible to correct TST for the effect of symmetry in the system? How to describe symmetry in transmission? How to include zero-point energy in classical trajectories? (SG)- New paradigm for studying Hamiltonian systems with steep potentials; chemical reactions are very far from being near-integrable, therefore, look at the billiard limit as a mathematical tool that allows mathematically rigorous studies. NHIM for the billiard system as an approximation to smooth Hamiltonian systems; include open billiards (VRK)- More complicated systems: What kinds of strange kinetics on dynamics have been observed in real systems as clusters or proteins?