**Searching for Reaction Coordinates and Order Parameters**

**Organizers:** Elber and Henkelmen

**TSRC Hosts:** Nana Naisbitt, 970-708-0004 and Rory Sullivan 970-708-4542

**Location:** Telluride Intermediate School, 725 W. Colorado Avenue

**Sunday, July 6**

6:00 – 8:00 Informal Meet and Greet at Arroyo Wine Bar and Gallery, 220 E Colorado Avenue, Cash Bar. TSRC employee will be on hand to answer questions.

**Monday, July 7**

8:45 – 9:15 Breakfast @ TSRC

9:15 - 10:30 **D. Zuckerman**

Exploring non-Markovian Analysis for the Weighted Ensemble and Beyond

10:45 – 12:00 **B. Peters**

TBA

12:00 – 1:00 Lunch @ TSRC

1:30 – 2:45 **Ron Elber**

 Exact Milestoning

2:45 – 4:00 **D. Perez**

 Accuracy of Kinetics in Coarse-Grained Molecular Dynamics

**Tuesday, July 8**

8:45 – 9:15 Breakfast @ TSRC

9:15 – 10:30 **P. Bolhuis**

 Path Sampling of Rare Event Networks

10:45 – 12:00 **H. Orland**

 Searching for Transition Paths

12:00 – 1:00 Lunch @ TSRC

1:30 – 2:45 **G. Henkelman** (with Sam Chill and Juliana Duncan)

A Comparison of Established and New Saddle Point Finding Methods

2:45 – 4:00 **L. Chen**

Hybrid Steered Molecular Dynamics Approach to Computing Binding Affinities

6:00 – 7:15 **TSRC TOWN TALK** at the Conference Center in Mouintain Village: “Lead us not into Hemptation: The genetics of the American Cannabis,” by George Weiblen, Distinguished Professor, University of Minnesota

**Wednesday, July 9**

8:45 – 9:15 Breakfast @ TSRC

9:15 – 10:30 **A. Voter**

 Local Hyperdynamics

10:45 – 12:00 **T. van Erp**

Reaction Rate Calculation using Path Sampling: Pitfalls and Opportunities

12:00 – 1:00 Lunch @ TSRC

1:30 – 2:45 **D. Makarov**

 Changing Reaction Pathways with Mechanical Forces

2:45 – 4:00 **C. Clementi**

Multiscale Characterization of the Photocycle of Photoactive Yellow Protein

6:00-8:00 Traditional TSRC Picnic at Ah Haa School for the Arts at 300 South Townsend. Family and guests welcome free of charge.

**Thursday, July 10**

8:45 – 9:15 Breakfast @ TSRC

9:15 – 10:30 **S. Huo**

 Issues in Dimensionality Reduction and Improvements

10:45 – 12:00 **J. Kaestner**

Minimum Free-Energy Paths Obtained from Umbrella Sampling

12:00 – 1:00 Lunch @ TSRC

1:30 – 2:45 **B. Leimkuhler**

 The State of the Art of the Timestep

2:45 – 4:00 **D. Theodoro**

 Energy Landscape Analysis of Atomic and Polymer Glasses

**Friday, July 11**

8:45 – 9:15 Breakfast @ TSRC

9:15 – 10:30 **C. Wong**

 Fast Models of Drug-Binding Kinetics for Drug Discovery

10:45 – 12:00 **C. Abrams**

**Meeting End**