Advanced Computational Physics

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- The energy landscape: properties and complexity (R. Ferrando)
  - Funnel-like and glassy potential energy surfaces
  - Inherent structure
  - Calculating the partition function: superposition appoximation
  - Transition rates: Transition State Theory, Kramers Theory

- Exploring the energy landscape: the global optimization problem (R. Ferrando)
  - Basics of Monte-Carlo and Molecular Dynamics simulations
  - Basin Hopping algorithm
  - Genetic algorithms

- Exploring the energy landscape: looking for saddle points (R. Ferrando)
  - Nudged Elastic Band method
  - Eigenvector Following

- Accelerated methods for exploring the energy landscape (F. Montalenti)
  - On-the-fly Monte Carlo
  - Hyperdynamics
  - Temperature Accelerated Dynamics
  - Parallel Replica Dynamics

- The free-energy landscape (G. Rossi)
  - Collective variables

- Sampling the free-energy landscape (G. Rossi)
  - Umbrella Sampling
  - Metadynamics