

Brainstorming Session #1

Brin Mathematics Research Center Workshop
Rare Events: Analysis, Numerics, and Applications

Prompts

- How to augment simulation with experiments for {free energy landscape / rare event / cryptic pocket / force field} prediction [Pilar, Greg, Bettina]
- Benchmark systems + community competitions (e.g., CASP, FLIP, TAPE) [Pilar]
- Incorporating dynamics as well as configurations into learning [Bettina, Dedi]
- Multi-well committers (e.g. 3-wells in 2D like a triangle) [Pilar]
- What are the 'big unsolved problems' in rare events? [Pilar]
- Special considerations for highly delocalized DOF (e.g., condensed phase systems) [Sapna] or high permutational symmetries (e.g., solvent) [Aaron]?
- Non-unit Jacobian determinants in learned low-dim CV projections [Bettina, Luke, Tony, Gabriel]
- Score-based models / diffusion models vs. GANs, VAEs, etc. in generative modeling [Eric, Grant]
- Modifying dynamics to speed convergence [Benoit, Bettina, Kostas, Katie, Andy]
- Rare events in deterministic dynamics where variability comes from initial conditions [Aaron]
- Non-Markovian models of conformational dynamics [Xuhui]