We want to accelerate or completely avoid MD simulations.

We want to quantify transitions.
CURRENT RESEARCH OF CAMERON’S TEAM


• Shashank Sule: Error analysis for diffusion maps-based approximations to the backward Kolmogorov operator.

• Christopher Moakler: analysis on complex chemical reactions arising in hydrocarbon pyrolysis with the aid of random graph theory.

• Lautaro Cilenti (Mechanical Engineering): Quantifying noise-driven transitions in coupled nonlinear oscillators with periodic forcing.
• Margot Yuan: Solving the backward Kolmogorov PDE by methods suitable for high dimensions based on neural network representations and tensor train representations.

• Manyuan Tao: modeling fracture in hydrogels — materials made up of networks of polymer chains and filled with water.

• Ryan Synk: making a path toward understanding and quantifying rare events in quantum systems.
WHAT WE WANT TO EXPLORE

- How one can use ML tools for quantifying rare events in stochastic systems
  - Solving PDEs in high dimensions by meshless methods
    - Neural networks, diffusion maps, tensor trains
  - Enhancing sampling by means of ML tools
  - Using graph data analysis
- To propagate to new areas (e.g. quantum systems)
- To understand basic physics in systems rare events can lead to catastrophic consequences (e.g. modeling fracture of hydrogels)
LOGISTICS
TWO TYPES OF TALKS

• Present your research

• Present a paper or several papers relevant to the topics of this RIT

TO EARN ONE CREDIT YOU NEED TO GIVE A TALK

REGISTRATION: AMSC689, SECTION 0802

ASK JESSICA SADLER TO ENABLE YOU TO REGISTER

WEBSITE: HTTPS://WWW.MATH.UMD.EDU/~EVANSAL/RIT.HTML
SOME SUGGESTIONS FOR PAPERS TO PRESENTS


- Haizhao Yang: https://haizhaoyang.github.io


- Pratyush Tiwary: https://sites.google.com/site/pratyushtiwary/, in particular, the paper on RAVE algorithm: https://aip.scitation.org/doi/10.1063/1.5025487
CALENDAR

- 02/11/2022
- 02/25/2022
- 03/04/2022
- 03/18/2022
- 04/01/2022
- 04/08/2022
- 04/22/2022
- 04/29/2022
- 05/06/2022