Machine Learnt Black Boxes for Physical and Materials Sciences

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Broad scope of computational molecular/materials sciences

- Solar energy conversion reactions
- Protein folding in cells
- Biological enzyme reactions
- Battery Applications
  - Anode (-)
  - Cathode (+)
  - Electrolyte

Involves black-box calculation of key quantities
- Energy $\mathcal{H}\Psi = E\Psi$
- Conductivity, Stiffness, Reactivity...

High Computational Cost
Studies involve many black-box evaluations, leading to $>10^6$ CPU costs

Data-Driven Strategy
- We will use available data to:
  1. Preserve accuracy
  2. Reduce computational cost
  3. Guide discovery

Dendrite formation at anode surface
- Design of electrolyte materials
Project Opportunities for CMS 273

- Project will explore systems at the classical, quantum, and continuum levels, using:
  - Gaussian Process Regression
  - Deep Neural Nets
  - Active Learning
  - Automated feature selection and refinement

- Want to learn more?
  - Talk to Kaushik or Tom directly or via email.
  - General overview: https://aip.scitation.org/doi/10.1063/1.5043213
  - Recent papers: DOI: 10.1021/acs.jctc.8b00636; arxiv.org/abs/1901.03309