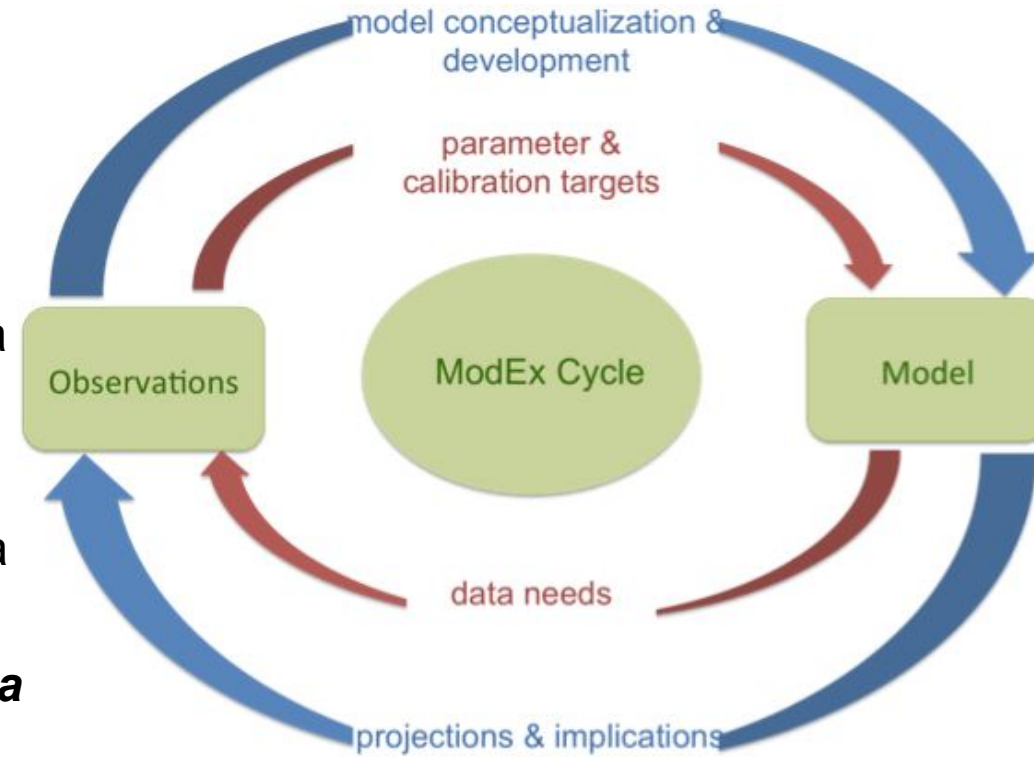




## Update on XAI for SARS-CoV-2 research

**Ben Brown, PhD**  
**Staff Scientist, EGSB**  
**May 7, 2020**

- 1) Evolution:** How are viral proteins co-evolving during the pandemic, and can we predict future mutations and the emergence of strains?
  - With Daniel Jacobson [ORNL], Patrick Chain [LANL]
- 2) Antivirals:** Can we design novel antiviral compounds with AI?
  - With Peter Nugent and Peter Zwart
- 3) TriP:** How does the **environmental microbiome** impact the transmissibility of the virus, and what interactions with policy and human behavior exist?
  - With Joshua Ladau, Matthias Hess [UCD], Katrina Abuabara [UCSF], Dan Jacobson [ORNL]
- 4) Climate:** How does **climate** impact...
  - With Eoin Brodie, Haruko Wainwright, Dan Feldman, Joshua Ladau, and team
- 5) ModEx: Can we take a data-driven “ModEx” approach to data collection and the design of interventions?**



- **Safety:** Computational Work == Pretty Safe (except for ergonomics!)
- **Scientific Highlights:**
  - 1) **Evolution:** Distribution of mutations has numerous higher-order dependencies – early results suggest a predictive model from sequence is possible, and may learn about protein complexes.
  - 3) **TriP:** The presence of fungal allergens may be protective – fitting machine learning models and working to collect enough confounding factors to convince ourselves.

