Workflows Combining Simulation and Experiment

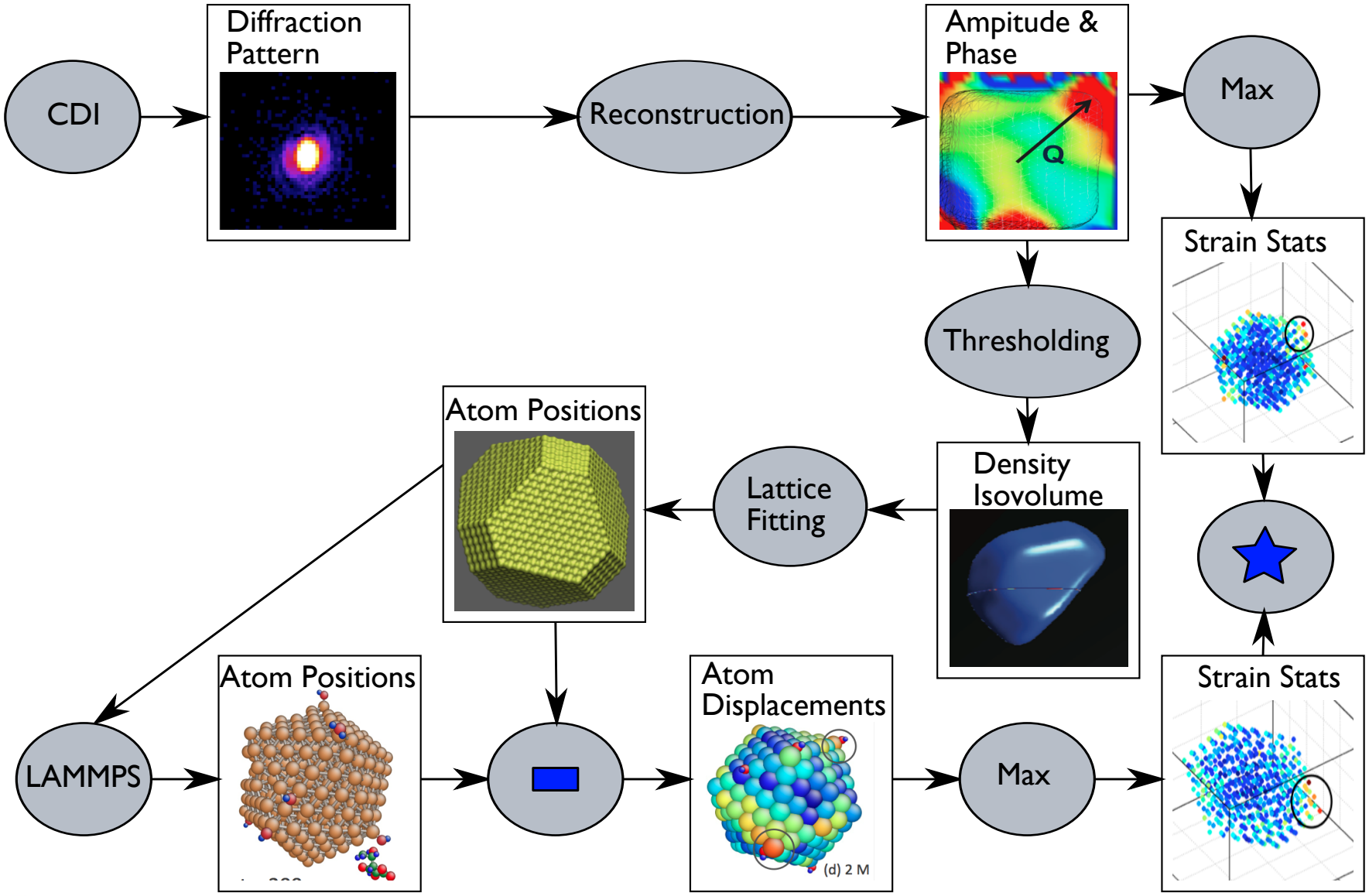
Tom Peterka
Mathematics and Computer Science Division
Argonne National Laboratory

SC15 BOF
Characterizing Extreme-Scale Computational and Data-Intensive Workflows
11/17/15

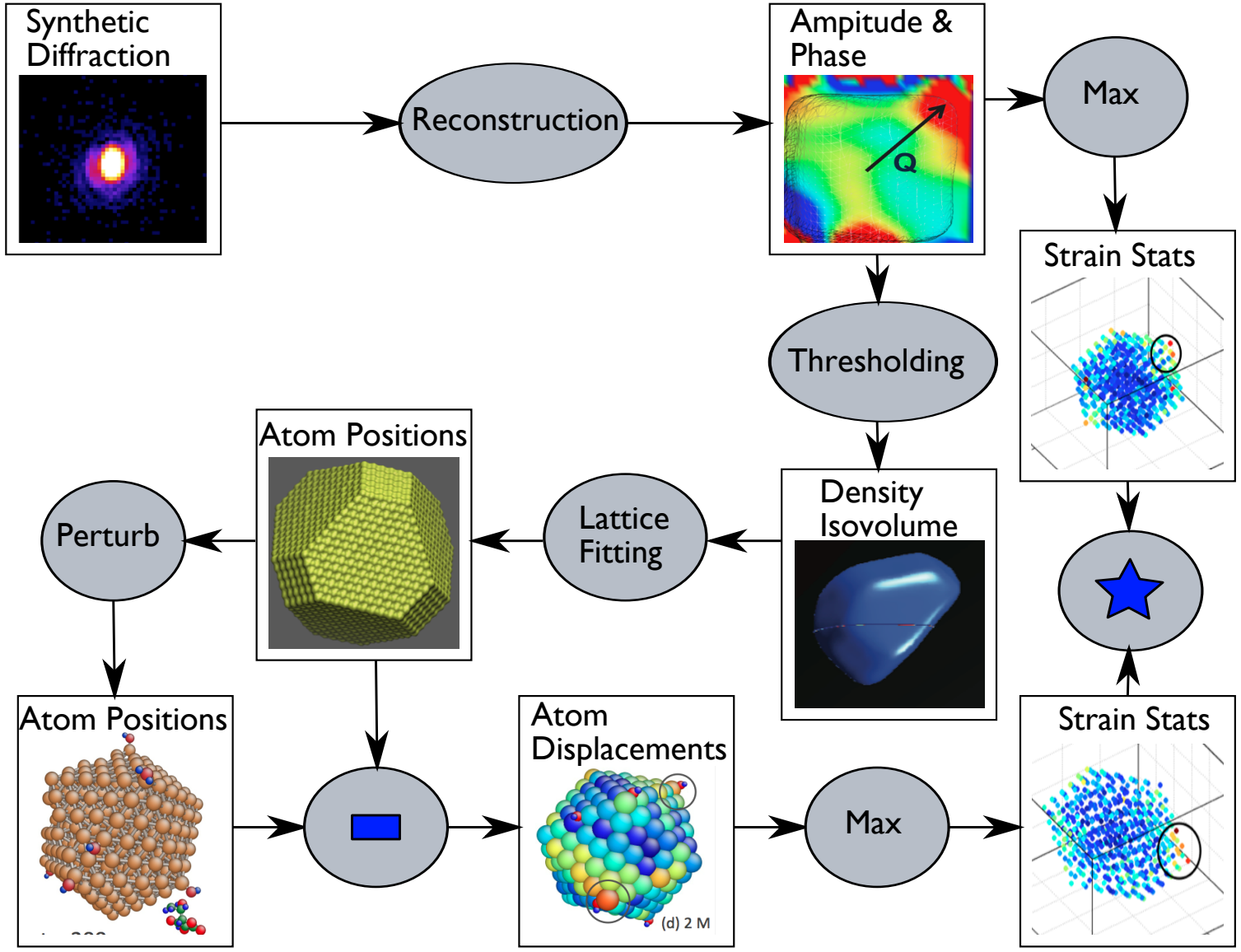
Introduction

- Motivation (physics, chemistry)
  - Experimental design
  - Simulation validation
  - New information
- Motivation (computer science, workflows)
  - Combine in situ w/ post hoc workflows
  - Combine HPC with DAC
  - Better coverage of science workflow by CS workflow
- Science examples
  - LAMMPS MD + synchrotron light source imaging
- Workflow examples
  - Forward problem
  - Reverse problem

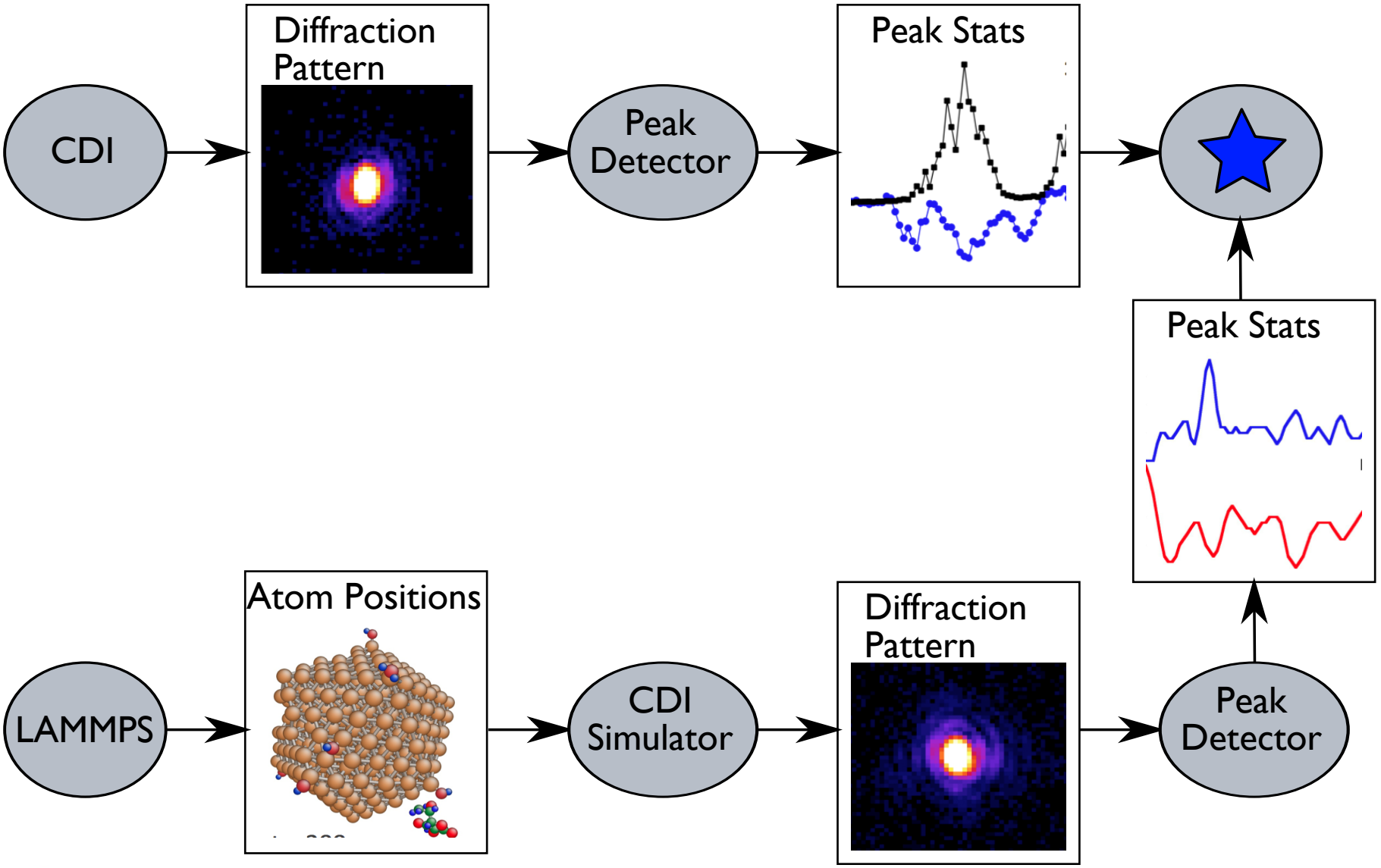
Forward Problem Full Workflow



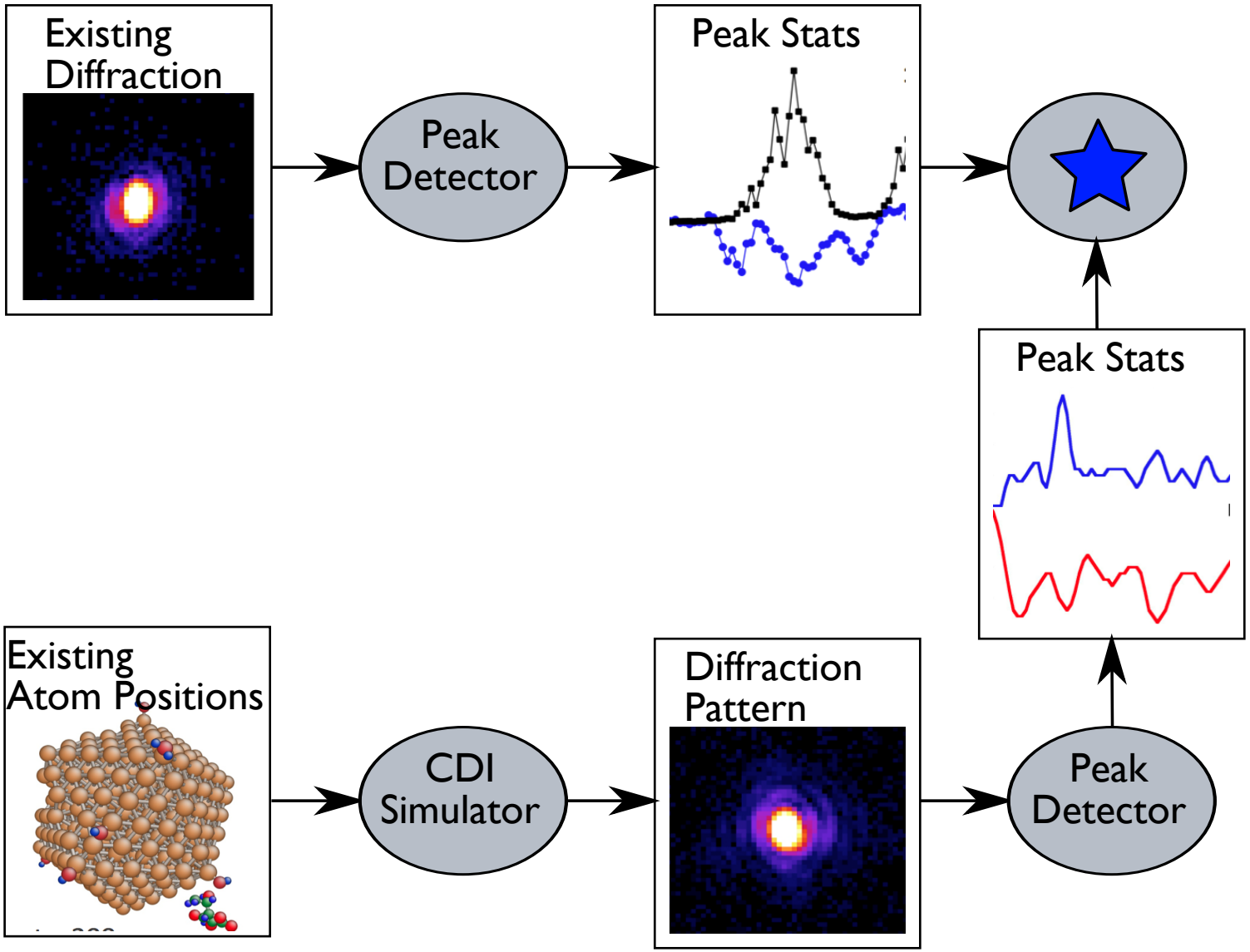
Forward Problem Mini Workflow



Reverse Problem Full Workflow



Reverse Problem Mini Workflow



Food For Thought

- Science workflow challenges
  - Time and space scales
  - http://tpeterka.github.io/maui-project/
- CS workflow challenges
  - Time latency between HPC and DAC parts of the workflow
  - Geographic distance between HPC and DAC
  - Provenance capture, reproducibility
- Mini workflow challenges
  - Synthetic data generation
  - Evaluation
- Other MD (simulation only) workflow examples
  - https://bitbucket.org/tpeterka1/decaf/
  - LAMPPS Decaf Example
  - Gromacs Decaf Example