

Workflows Combining Simulation and Experiment

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SC15 BOF

Characterizing Extreme-Scale Computational and Data-Intensive Workflows

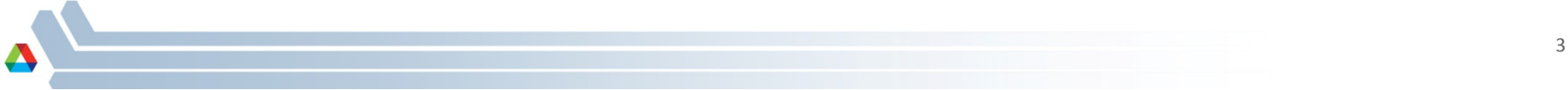
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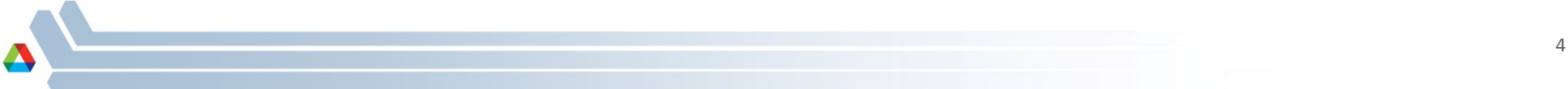
Introduction

- 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

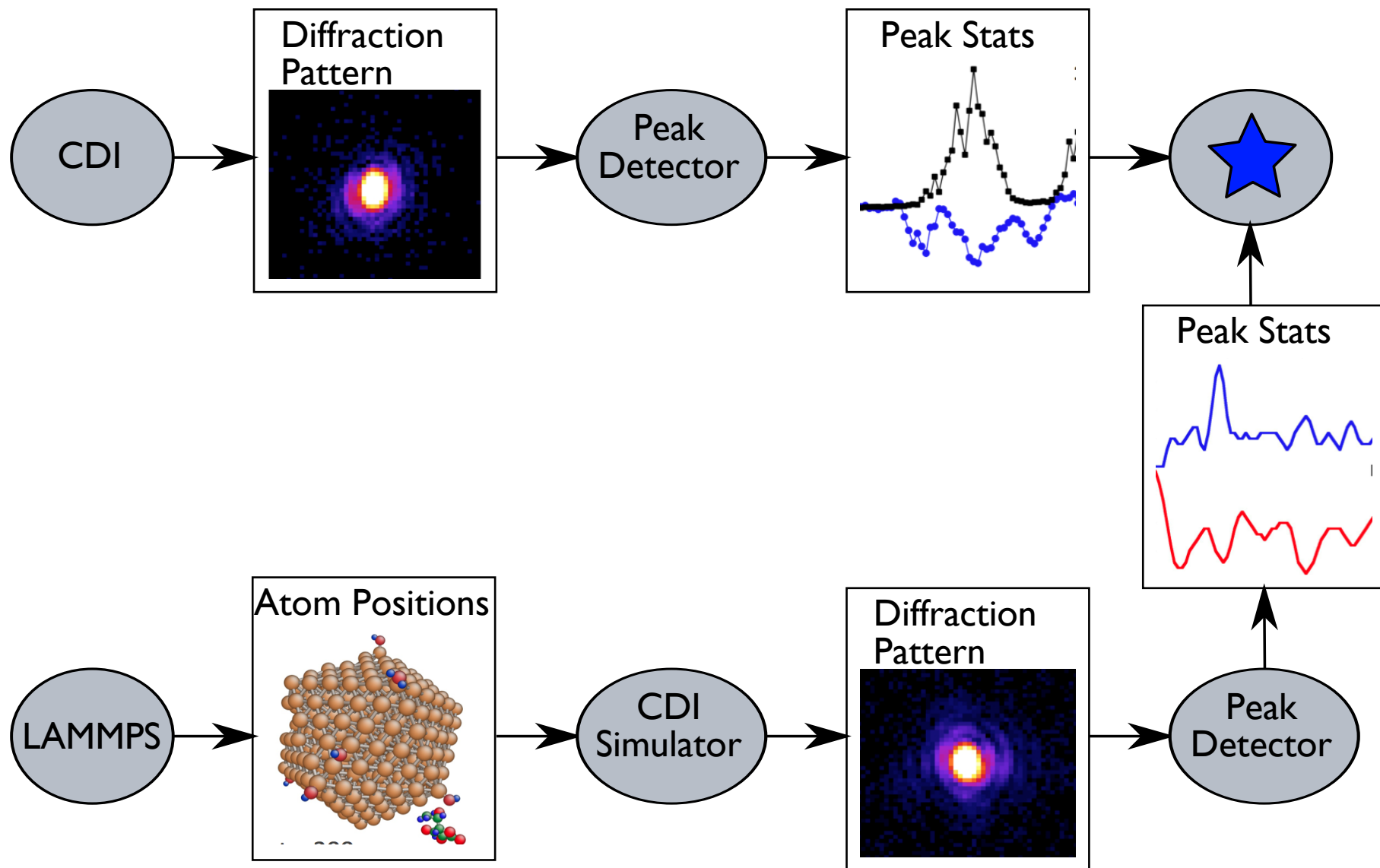


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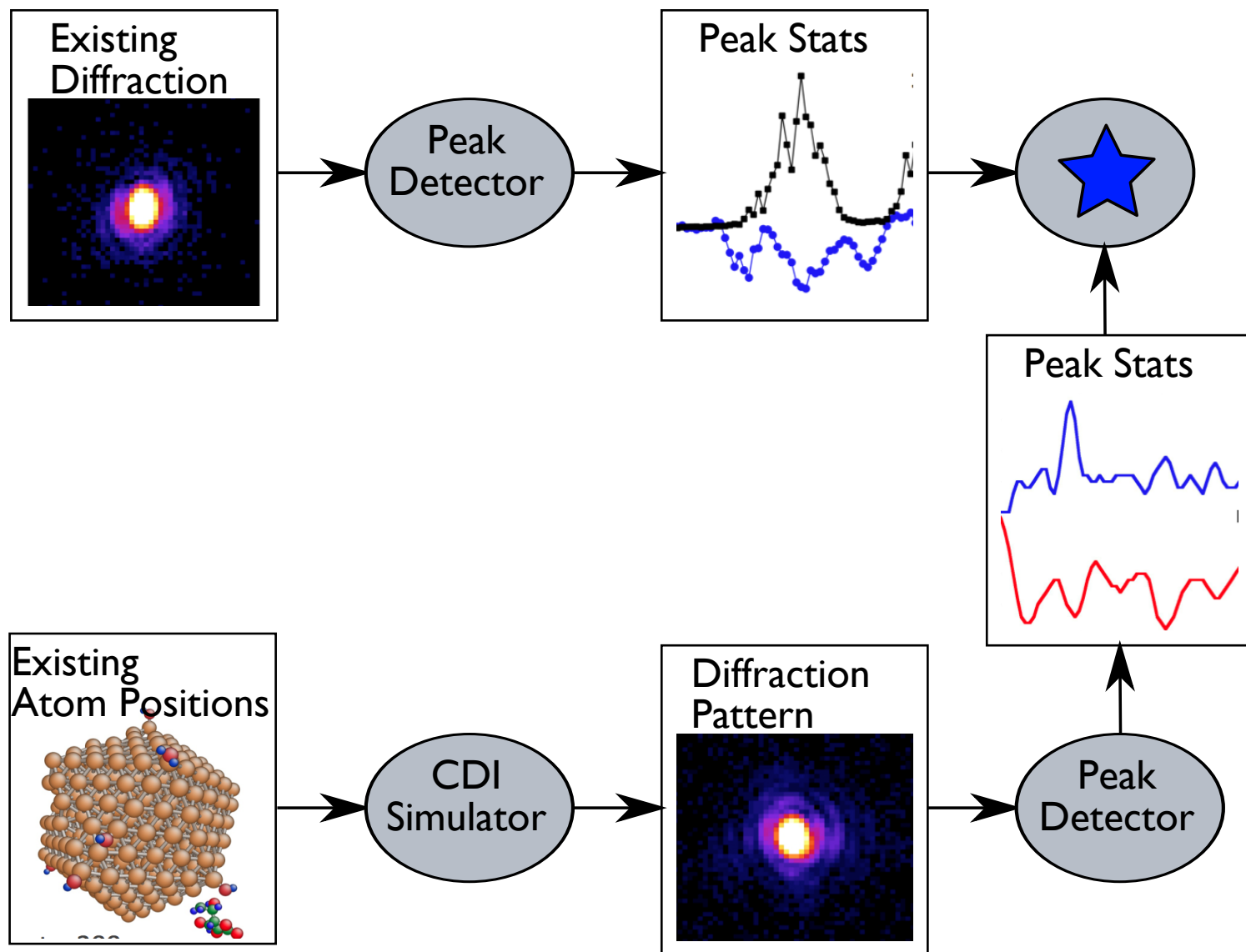




Reverse Problem Full Workflow



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

