Workshop on Computational and Autonomous Workflows (CAW)
ORNL

July 14, 2020

Speaker:

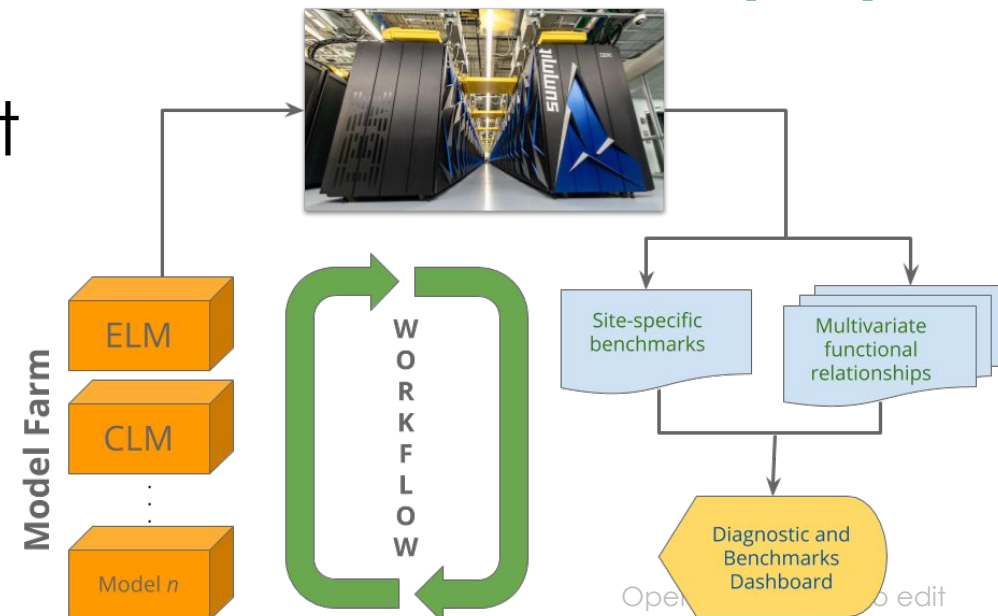Forrest M. Hoffman
Computational Earth Sciences Group

1. Describe a day in the life of an ORNL scientist in your area in terms of a typical end to end workflow to do your science

- In the Computational Earth Sciences Group, we improve process understanding of the global Earth system by
  - developing and applying models, machine learning, and computational tools at scale;
  - integrating observational data;
  - and quantifying Earth system predictability and uncertainty associated with interactions between water, energy, biogeochemical cycles, and aerosols
- In practical terms, we
  - develop numerical methods and program code on HPC
  - conduct simulations of Earth system models and regional climate models
  - analyze, evaluate, and benchmark simulations, often in comparison with in situ, remote sensing, and reanalysis data

OAK RIDGE
National Laboratory

2. What are the current challenges you face in your workflow?

- Developing model code with performance portability across architectures with and without accelerators
- Analyzing and synthesizing data from a wide variety of sources in a wide variety of formats for use in evaluating models
- Developing new analysis and scoring methodologies for benchmarking component models (atmosphere, land, ocean, sea ice, and land ice)
- Conducting simulations of multiple models across multiple platforms that produce different equilibrium states, and benchmarking model results through comparison with obser-vational data at multiple scales

Land Model Testbed (LMT)

Model Farm

ELM

CLM

Model *n*

WORKFLOW

Site-specific benchmarks

Multivariate functional relationships

Diagnostic and Benchmarks Dashboard

OAK RIDGE
National Laboratory

3. Discuss opportunities for collaboration for ORNL workflow researchers

- Integrating complex model coupled model configuration, initialization, spin-up, and large simulation experiment execution on all HPC environments across institutions with Jupyter Notebooks / Jupyter Hub
- Integration of post-processing, benchmarking, and visualization with model assessment dashboards across multiple evaluation packages with Jupyter Notebooks / Jupyter Hub
- Completely automated retrieval of simulation experiment output (10s of TB) from HPSS and ESGF across all institutions from within Python analysis tools
- Writing and submitting manuscripts to *Nature* and *Science*

OAK RIDGE
National Laboratory