Towards Diversified Exascale NWP Workflows

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ECMWF Workshop on HPC in Meteorology - Oct 10, 2023, Bologna, Italy

Acknowledgements

This work is funded by the NOAA Software Engineering for Novel Architectures (SENA) Program

In collaboration with U.S. Department of Energy Exascale Computing Project & Parallel Works (funded by DOE Small Business Innovation Research)

Supported by NOAA Research and Development HPC (RDHPCS) Program

Special thanks to: Todd Munson, Eric Schnepp, James Corbett, Jim Garlick

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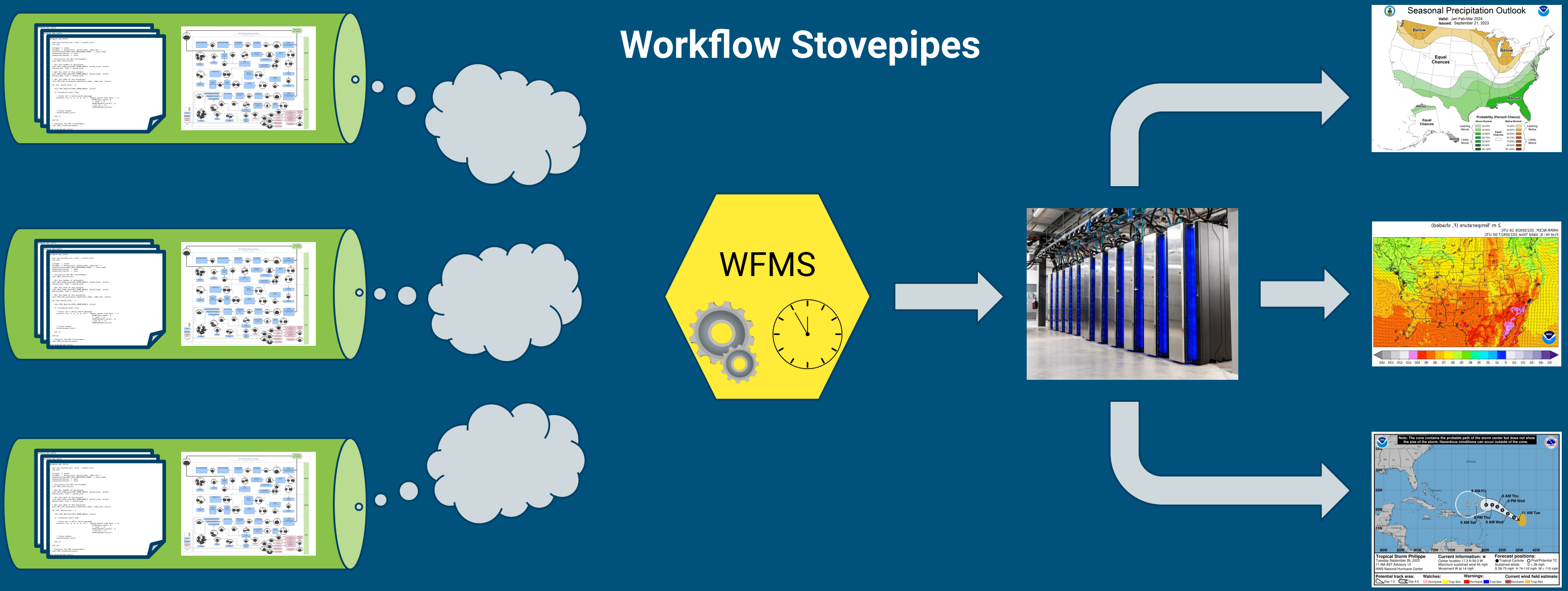
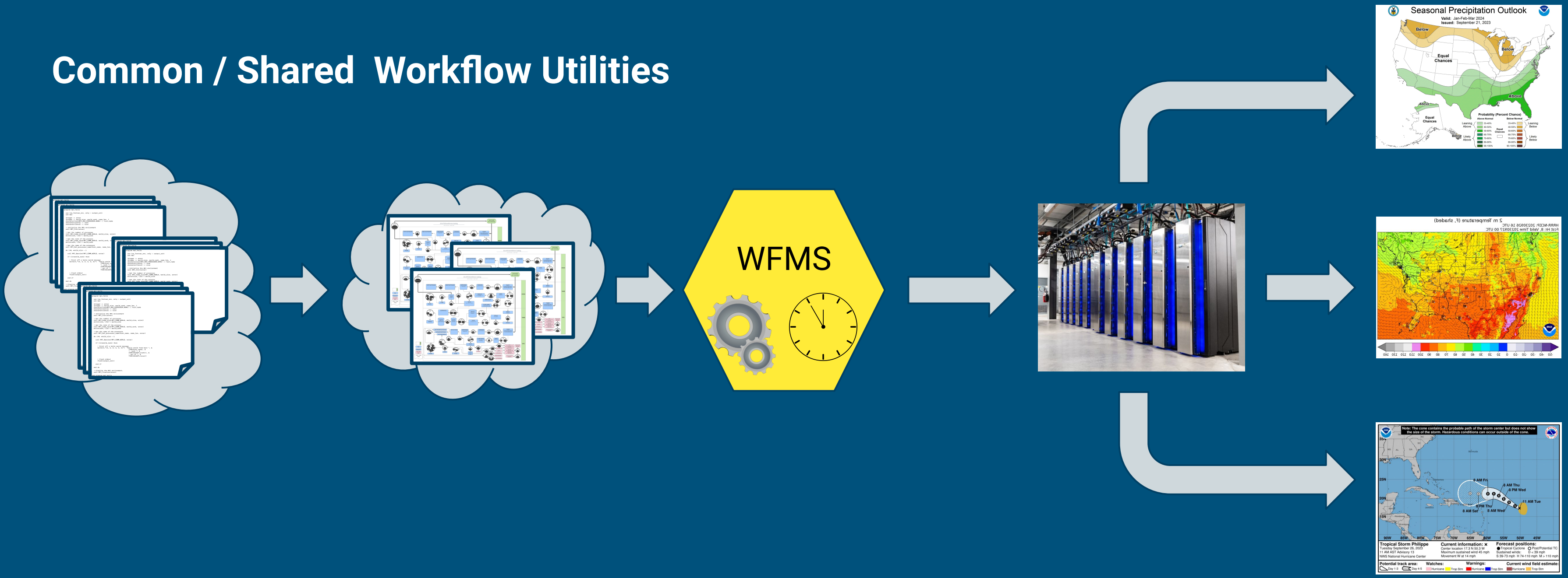
The Dark Ages

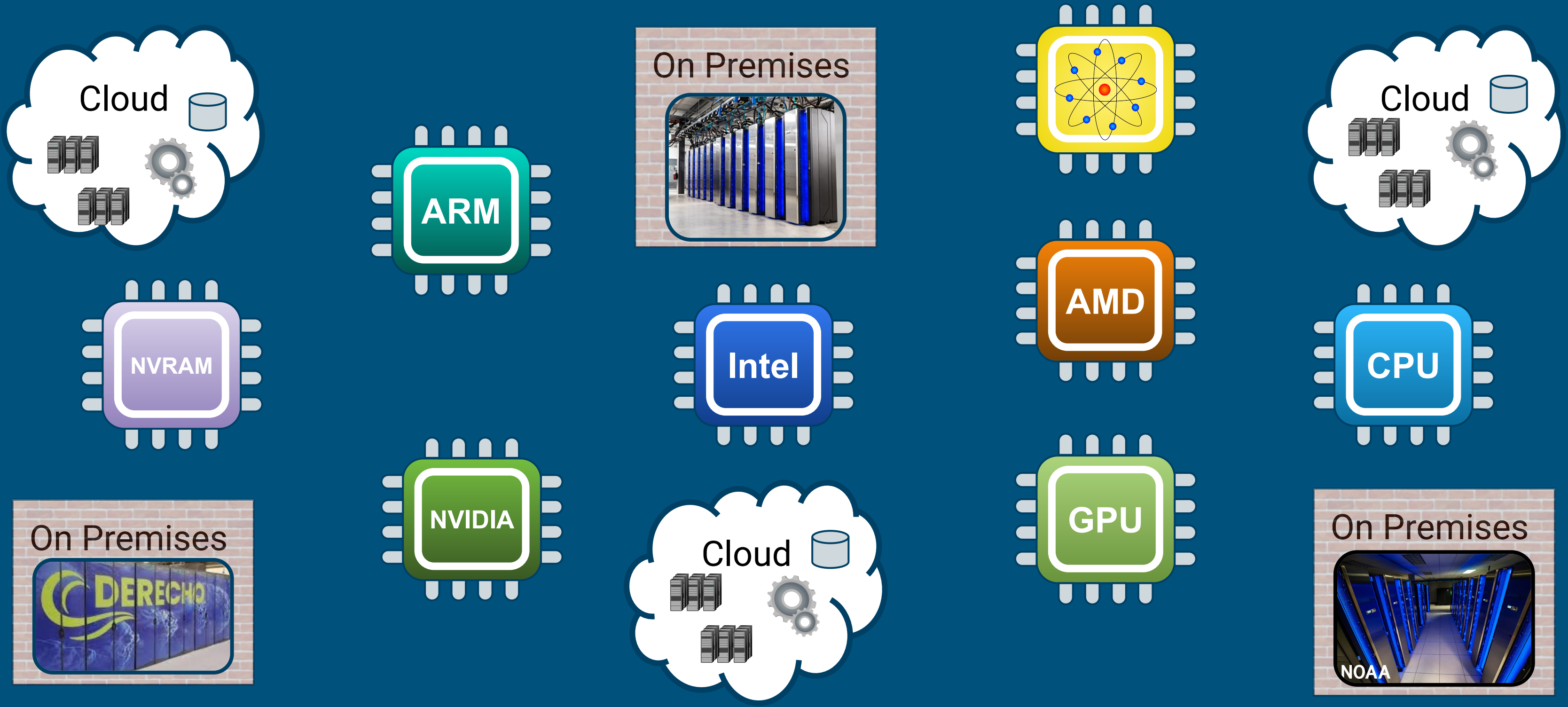


The (Unification) Enlightenment

Common / Shared Workflow Utilities



A Diversification Disruption



A Diversification Disruption

- The HPC landscape is changing
  - Diversification of hardware architectures
  - Diversification of programming models
  - Diversification of computational methods
  - High Throughput Computing (HTC) growing in importance
- Applications are changing
  - Diversification of components and services
  - Scaling up and out for capacity and access to diverse resources
  - Core services may be distributed or only available in certain places
  - Collaboration and sharing of data and products

A Tale of Two Workflow Regimes

R2O Pipeline

- Transition NWP Research to Operations
- Run the Operational system in Research environment
- Conform to requirements at the bottom of the “funnel”
- Use Operational workflow to make incremental forecast quality improvements

Features

- Operational mission is difficult - many modeling systems
- “Funnel” requirements evolve very slowly and meticulously
- Extremely risk averse
- Workflows are a means to an end – A tool in the toolbox

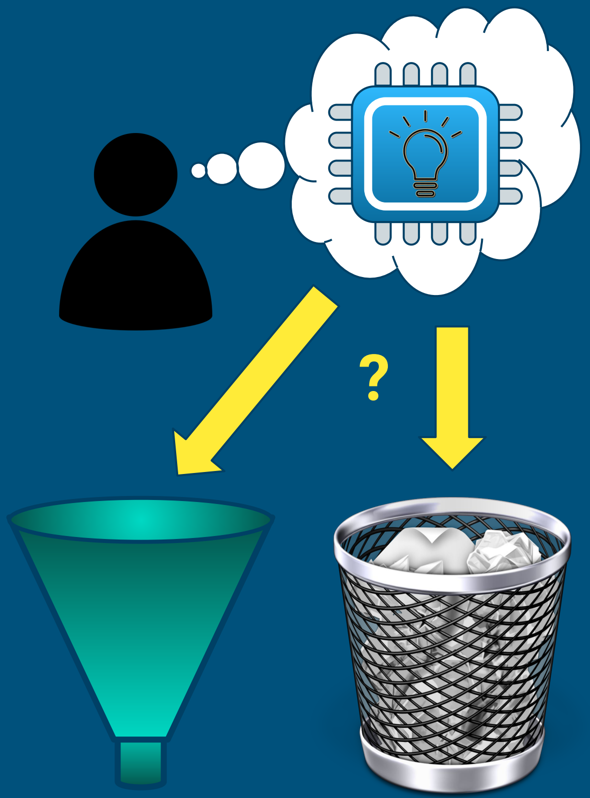
A Tale of Two Workflow Regimes

Long Range HPC (Exascale) Research

- Test and explore viability of emerging technologies
- Adapt the Operational system to use new technologies
- R2O “funnel” requirements lack the necessary agility & flexibility
- Develop workflows that apply HPC advancements to NWP

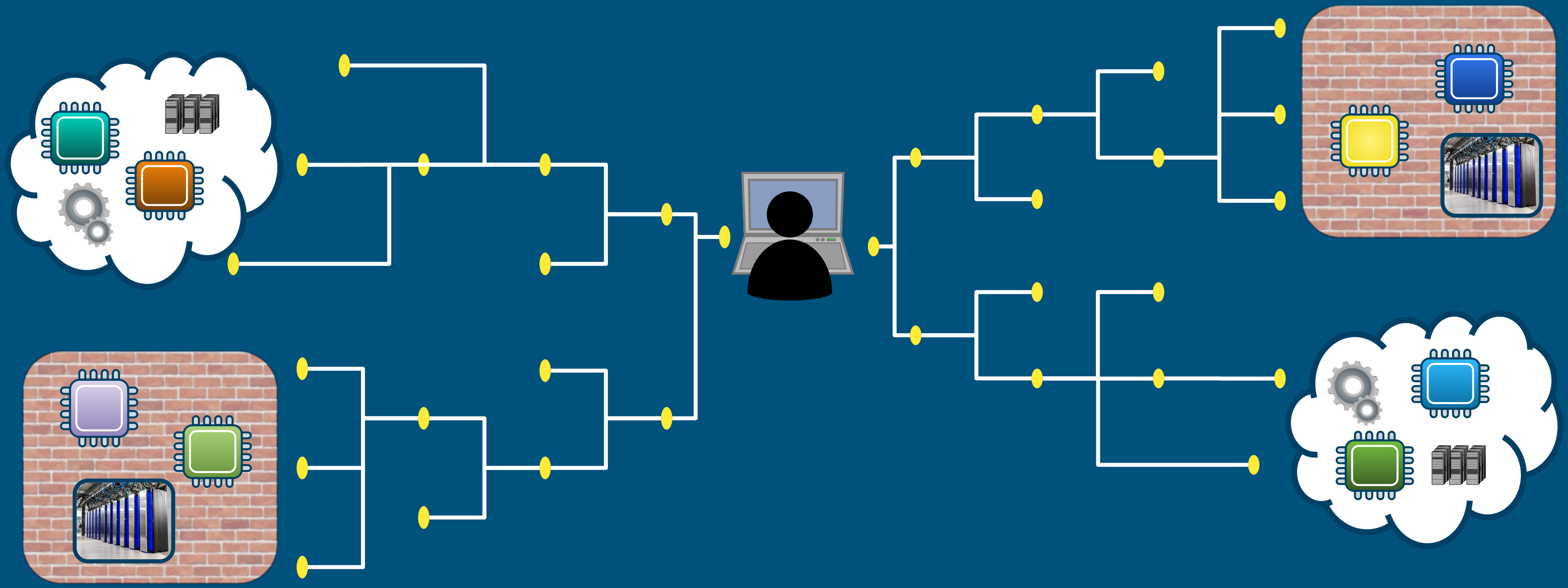
Features

- Diversification of HPC presents many challenges
- “Funnel” requirements inhibit “out-of-the-box” exploration
- Accept risk of using tools not currently available in Operations
- Diversified workflows are the product of the research



Our Vision

Diversified distributed workflows to enable NWP HPC Research



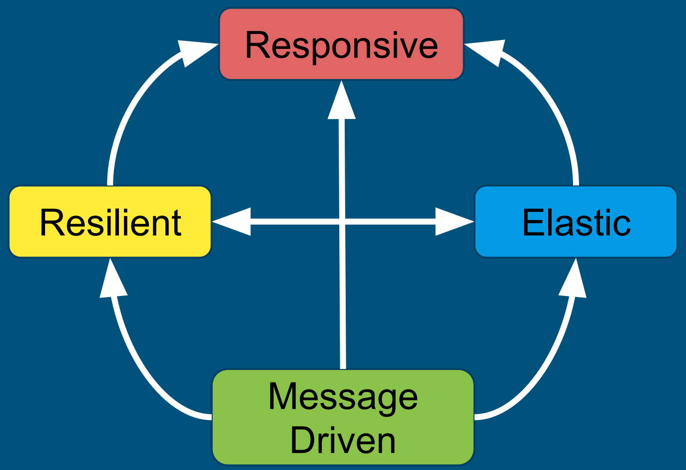
Guiding Principles

- Seamlessly distributed NWP application workflows
- Use existing, hardened, exascale-ready, tools
- Use UFS Unified Workflow building blocks
- No privileged access required for installation or use
- Configuration fully decoupled from execution
- “Let it fail” design for service lifecycle management

Inspiration From The Reactive Manifesto

Properties of reliable distributed applications

- **Responsive** - Consistent, rapid, response times to user requests
- **Resilient** - Maintain responsiveness during failure with isolation, replication, and delegation of failure recovery
- **Elastic** - Stay responsive under varying workloads by scaling resources and designing without points of contention
- **Message Driven** - Asynchronous, location transparent, messaging, between loosely coupled, isolated, components



Which Tools Should We Use?

A Scientific Workflow Management Community Challenge

Massive proliferation of bespoke workflow systems

ExaWorks

Democratize access to hardened, composable HPC workflow tools

- PSI/J
- Flux
- Parsl
- RADICAL
- Swift/T

Support for MPI

Portable Python-based workflow expression with multiple executors for different back-ends

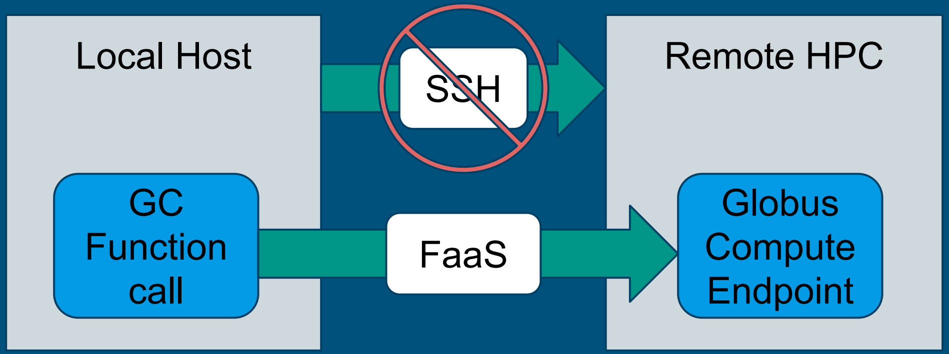
Which Tools Should We Use?

A Distributed Computing Challenge

Reliable management of secure communications between remote systems

Globus Compute

Secure function as a service (FaaS) for remote, high performance, “fire and forget” execution



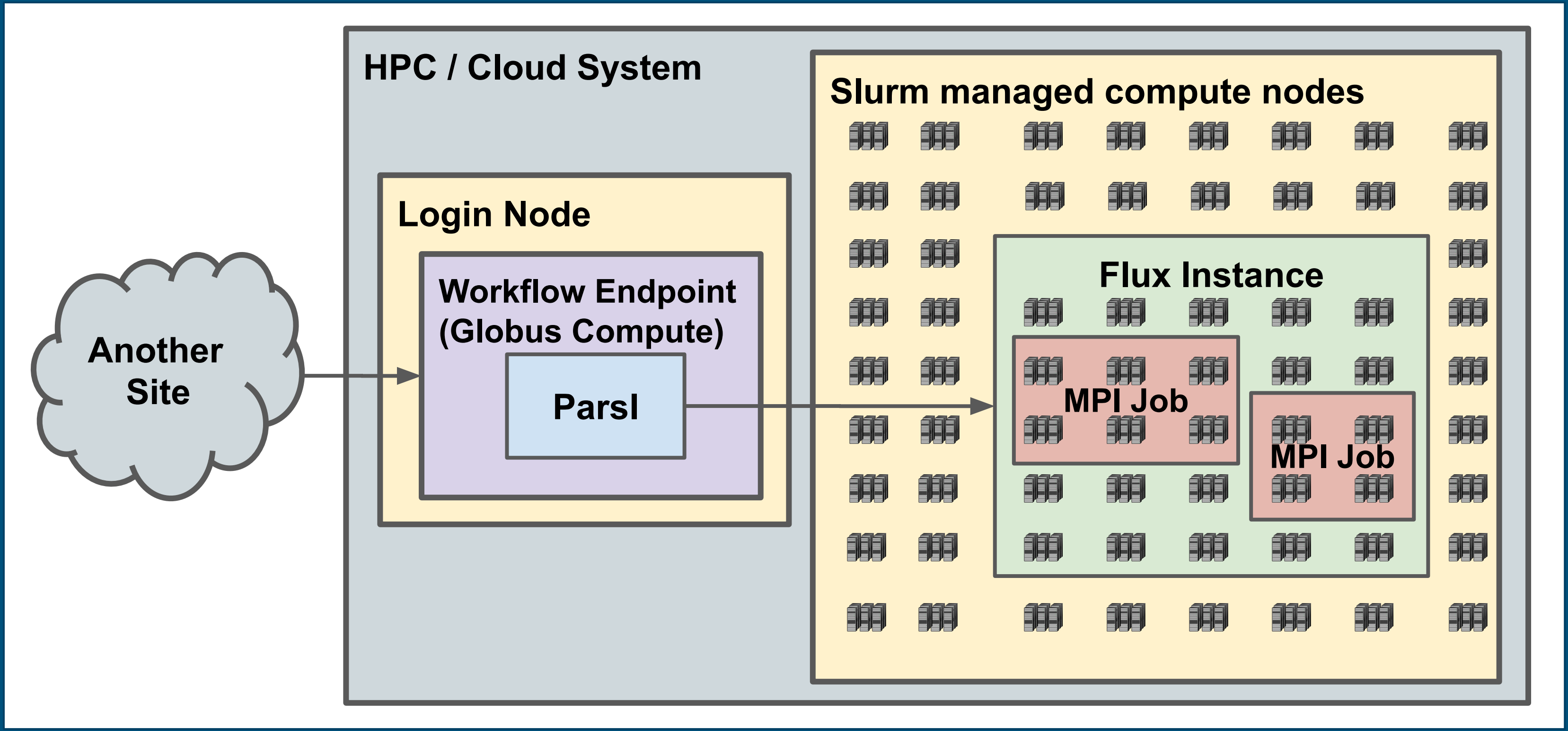
More Challenges

- Should workflows be expressed as programs or as configurations?
  - Python or YAML?
- What about the data?
  - How and when should we move it?
  - Flexible slice and dice - ECMWF Polytope data cube access?
  - Egress and storage costs
  - Globus Flows for multi-hop transfers?

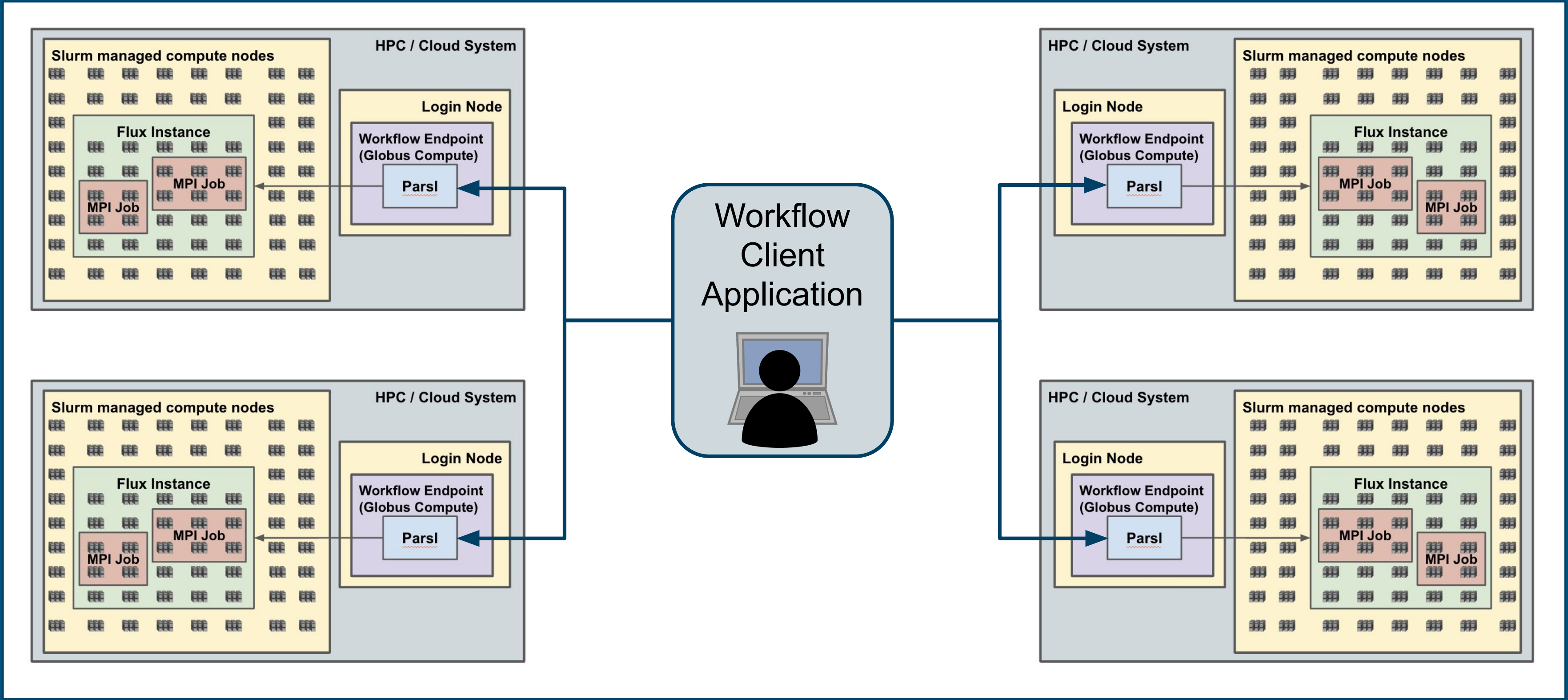
More Challenges

- How do we monitor and steer distributed workflows to diagnose problems?
  - If a workflow is a Python program, how do you interrogate and control it?
  - EPMT: The GFDL Experiment Performance Metrics Tracking Infrastructure
- How do we test while developing distributed workflow capabilities
  - Requires large, complex supporting software stacks
  - CI / CD using containerized Slurm clusters
  - Globus client credentials with GitHub secrets

The Current Architecture



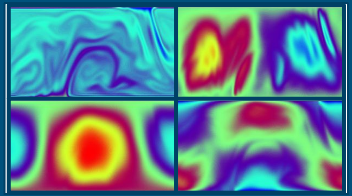
The Current Architecture

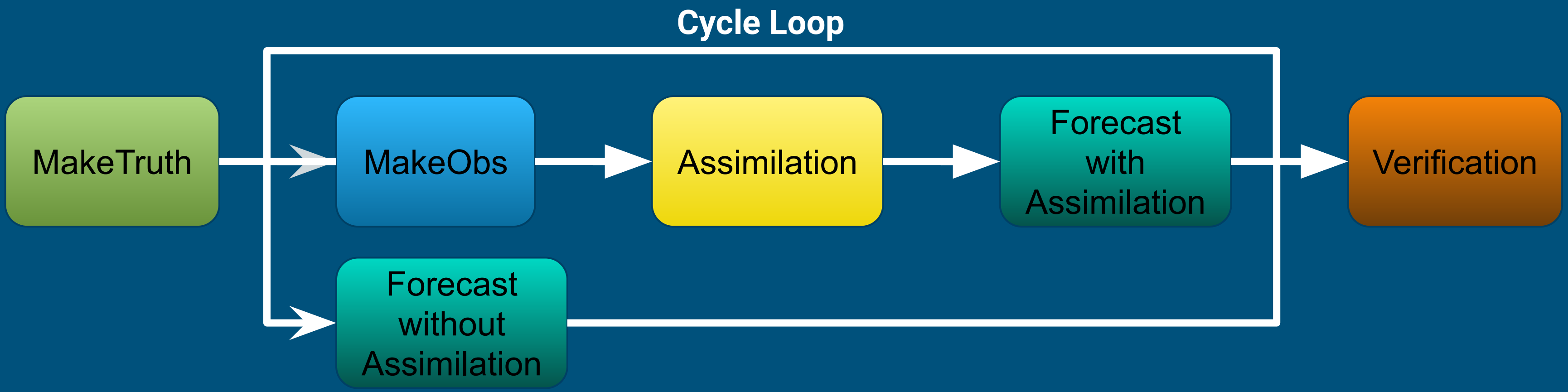


The Test Application

Cycled Data Assimilation with JEDI's Quasi-Geostrophic (QG) Model

- Start with 3D/4D variational methods
- Progress to fully distributed 3D/4D EnsVar ensembles





The Test Application

```
# Define "truth" forecast task
@bash_app
def truth_run_app(jedi_path, stdout=None, stderr=None, parsl_resource_specification={}):
    return '''
    export JEDI_PATH={}
    . $JEDI_PATH/bin/setupenv-hercules.sh
    unset I_MPI_PMI_LIBRARY
    $JEDI_PATH/bin/qg_forecast.x $JEDI_PATH/yaml/truth.yaml
    '''.format(jedi_path)
```

```
# Run the truth forecast
truth = truth_run_app(jedi_path='/path/to/JEDI',
                      stdout=os.path.join(jedi_path, 'truth.out'),
                      stderr=os.path.join(jedi_path, 'truth.err'),
                      parsl_resource_specification={"num_tasks": 1, "num_nodes": 1}
                      ).result()
```

Summary Remarks

- We have a vision, and many questions, but do not yet have all the answers
- We are testing Parsl + Flux + Globus Compute
  - Parsl → High throughput computing and powerful programming interface
  - Flux → MPI-aware scheduling within Parsl workflows
  - Globus Compute → Function as a service (FaaS) for secure distributed execution
- We are starting small for testing and exploration purposes
  - Simple JEDI QG data assimilation workflow
- We are making use of UFS Unified Workflow development where possible
- Demonstration with a “real” model once foundational pieces are settled

Questions / Discussion