Design of a Generic Workflow Generator for the JEDI Data Assimilation System

Mark Olah and Yannick Trémolet

Joint Center for Satellite Data Assimilation (JCSDA)

molah@ucar.edu

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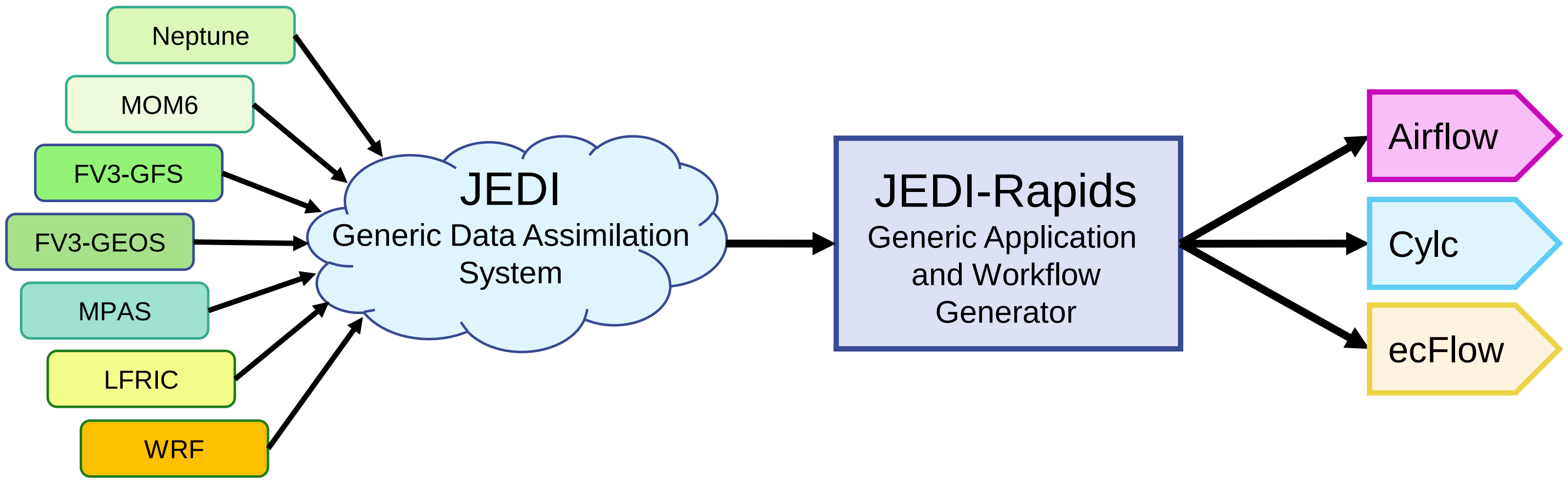


JEDI: Joint Effort In Data Assimilation Integration

Partner Organizations

- NOAA
- US Navy
- US Air Force
- NASA [EMC]
- NCAR
- UK Met Office

JEDI Core Team

- Lead: Yannick Trémolet
- ~10 FTE Programmers
- Boulder, CO; Greenbelt, MD; France
- Organized < 2 Years Ago

Agile Development Philosophy

- Git; Github; Git LFS; Git-flow; ZenHub
- Core Languages: C++ and Python
- CMake; ecBuild Bundles
- Automated Testing [CI]
  - CTest, Codecov, CDash, Valgrind
  - TravisCI; AWS CodeBuild
- Containers:
  - Docker, Singularity, Charlie Cloud
- Cloud computing
  - Storage, Compute, Automation, Hosting

Reproducibility in Scientific Applications

Bitwise Reproducibility

- Not generally achievable
- Severe implications for performance
- Inhibits portability
- Requires static, isolated systems
- Slows the pace of development

Scientifically Meaningful Reproducibility

- Realistic floating point tolerances
- Tolerate benign permutations / ordering
- Handle unexpected events / Avoid failures
- Enhances collaboration
- Aids the pace of development

Desirable Types of Reproducibility

Portability of Runtime Environment

- Temporal reproducibility (single system)
- Reproducibility over processor/node counts
- Reproducibility between Machines
- Reproducibility between Compilers / MPI
- Reproducibility between Operating Systems

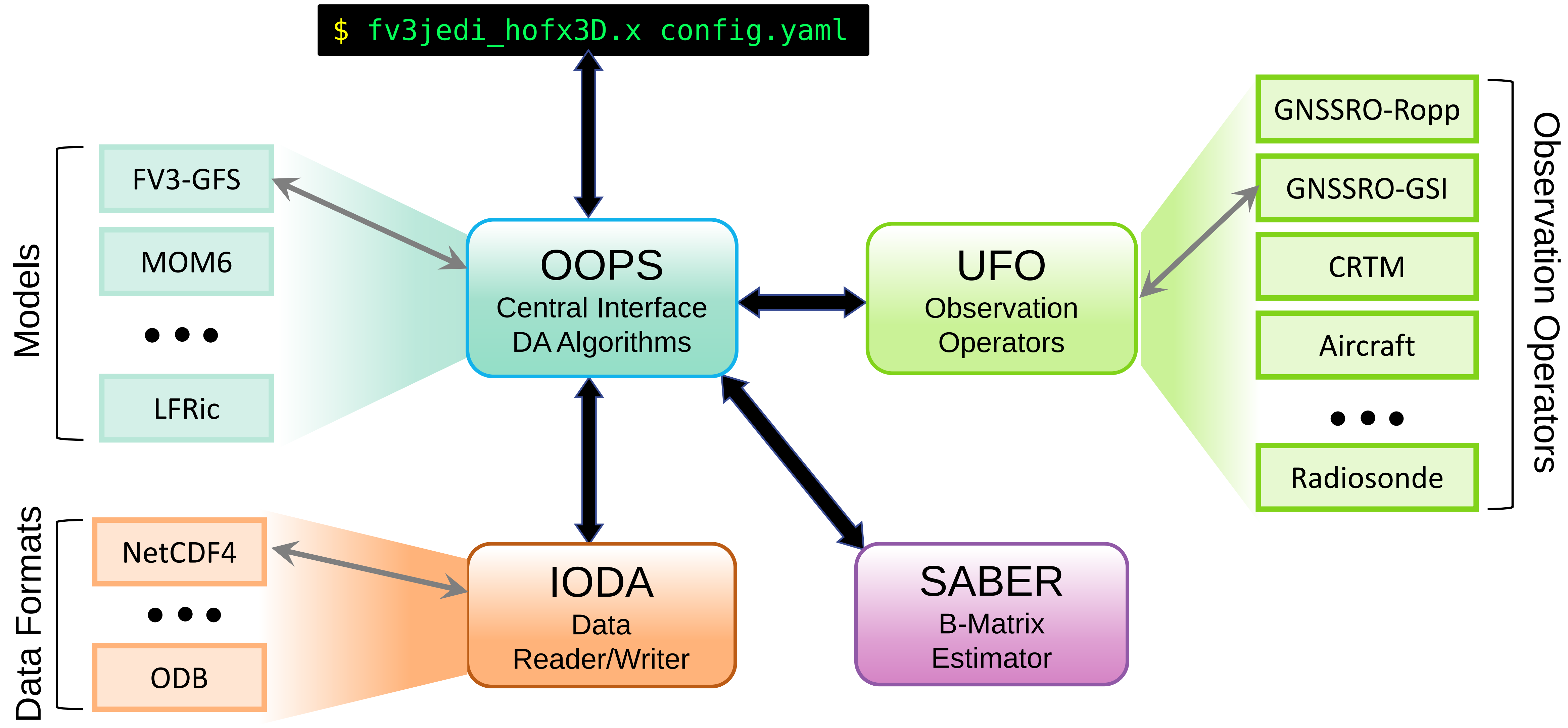
Portability of Algorithmic Environment

- Reproducibility between Problem Scales
- Reproducibility in Performance Characteristics
- Reproducibility of Algorithms Across Models
- Composability of components and interfaces
- Adaptability to dependency updates

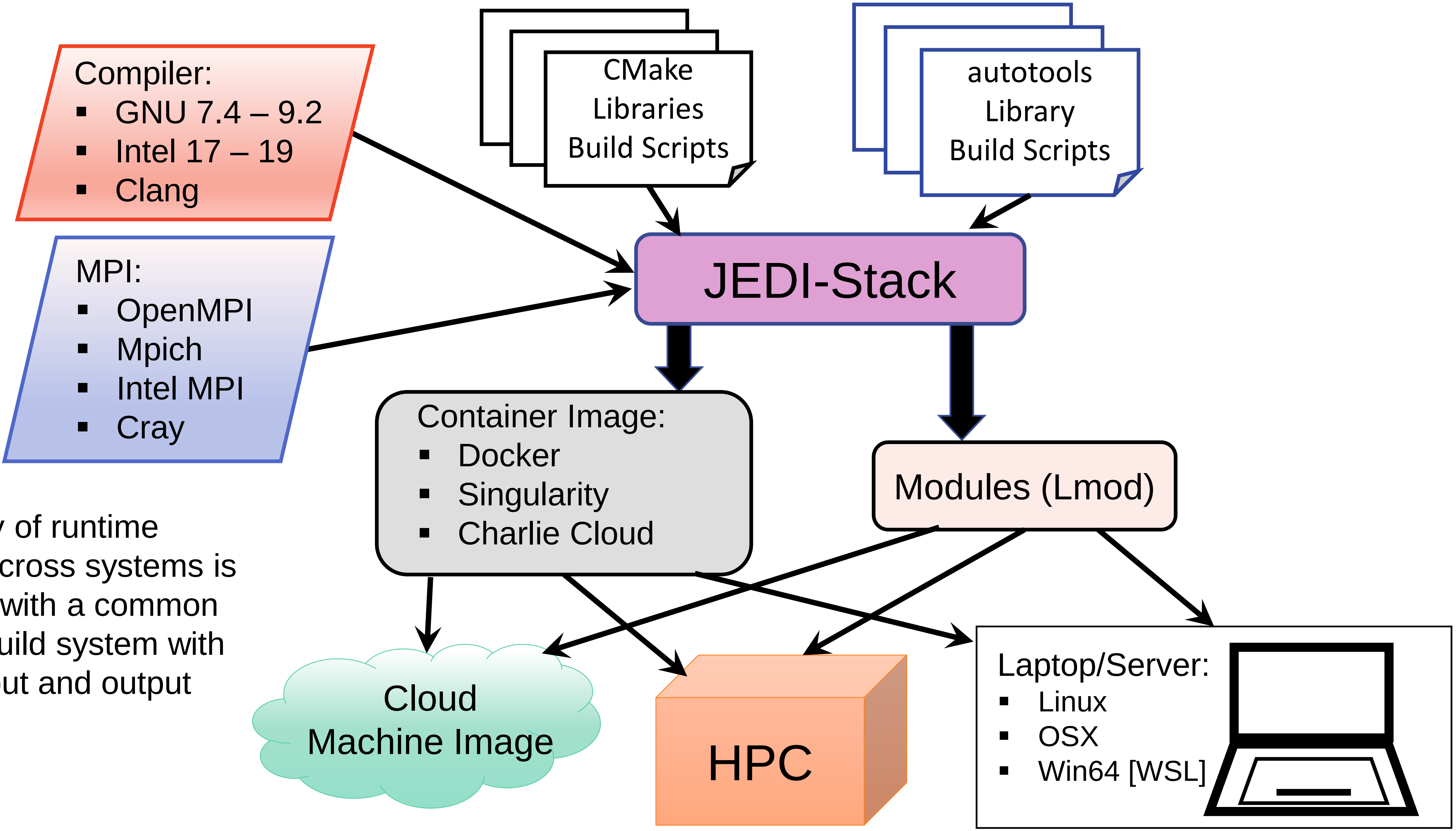
Implications of Full Runtime Portability for JEDI

- Need to move between workstation and Cloud and amongst varying HPC Environments
  - Must package and provide necessary dependencies
- Free and Open-source libraries and tools
  - Proprietary dependencies can be used but not required
- Easily adapt applications to different workflow engines
- Prefer universal, open source data formats.
- Data products must be available to all partners and collaborators
- Build systems must be cross-platform and adapt to wildly different systems
- Generic interfaces

JEDI DA System: Generic Interfaces



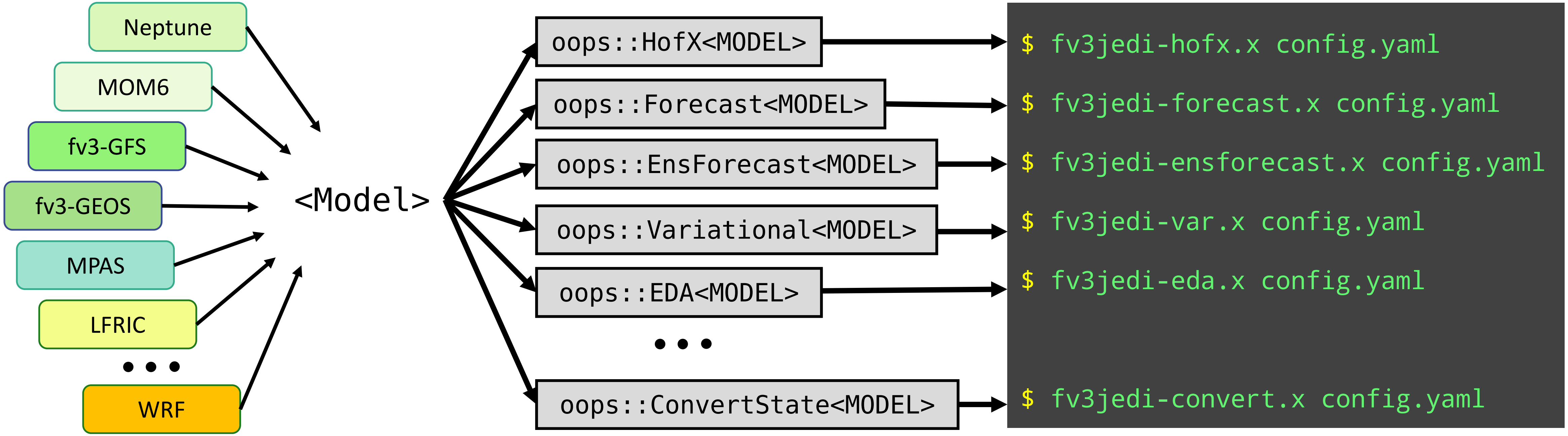
JEDI Runtime Environment Portability



Reproducibility of runtime environment across systems is accomplished with a common dependency build system with flexibility in input and output configuration.

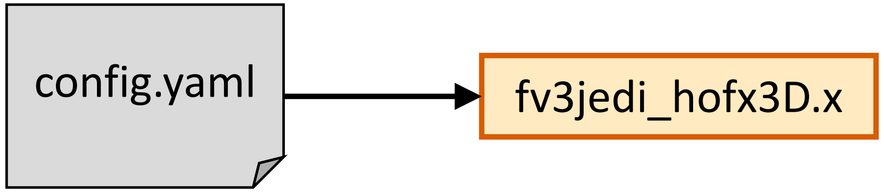
JEDI Workflow System Structure

- The JEDI system is generic with respect to Model, but presents a common interface
  - Each model produces the same fundamental set of executables
  - Each executable takes a single YAML file as input
  - GOAL: Mirror this structure in overall workflow structure and guidelines



JEDI Generic Executable Interfaces

```
$ fv3jedi_hofx3D.x config.yaml
```



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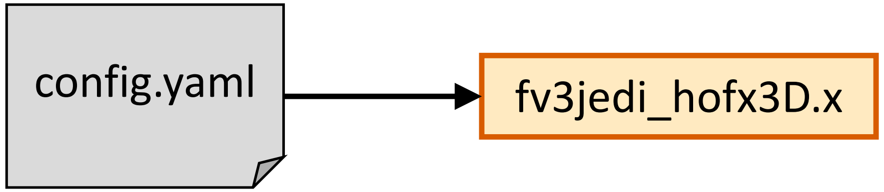


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Assimilation Window:
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  Length: PT6H
Geometry:
  nml_file: Data/fv3files/input_gfs_c768.nml
  trc_file: Data/fv3files/field_table
  pathfile_akbk: Data/inputs/gfs_c768/akbk-gfs.nc
Initial Condition:
  filetype: gfs
  datapath_tile: Data/inputs/gfs_c768.20190709.00/
  filename_core: 20190709.060000.fv_core.res.nc
  filename_trcr: 20190709.060000.fv_tracer.res.nc
  filename_sfcd: 20190709.060000.sfc_data.nc
  filename_sfcw: 20190709.060000.fv_srf_wnd.res.nc
  filename_cplr: 20190709.060000.coupler.res
  variables: ["T","DELP","sphum","phis"]
Observations:
  ObsTypes:
  - ObsSpace:
      name: GnssroBndROPP2D
      ObsDataIn:
        obsfile: Data/obs/cosmic1/KOM5_20190709_06Z.nc
      ObsDataOut:
        obsfile: Data/hofx/hofx_gfs_c768_gnssro_ropp2d_KOM5_20190709_06Z.nc4
      simulate:
        variables: [bending_angle]
    ObsOperator:
      name: GnssroBndROPP2D
      ObsOptions:
Prints:
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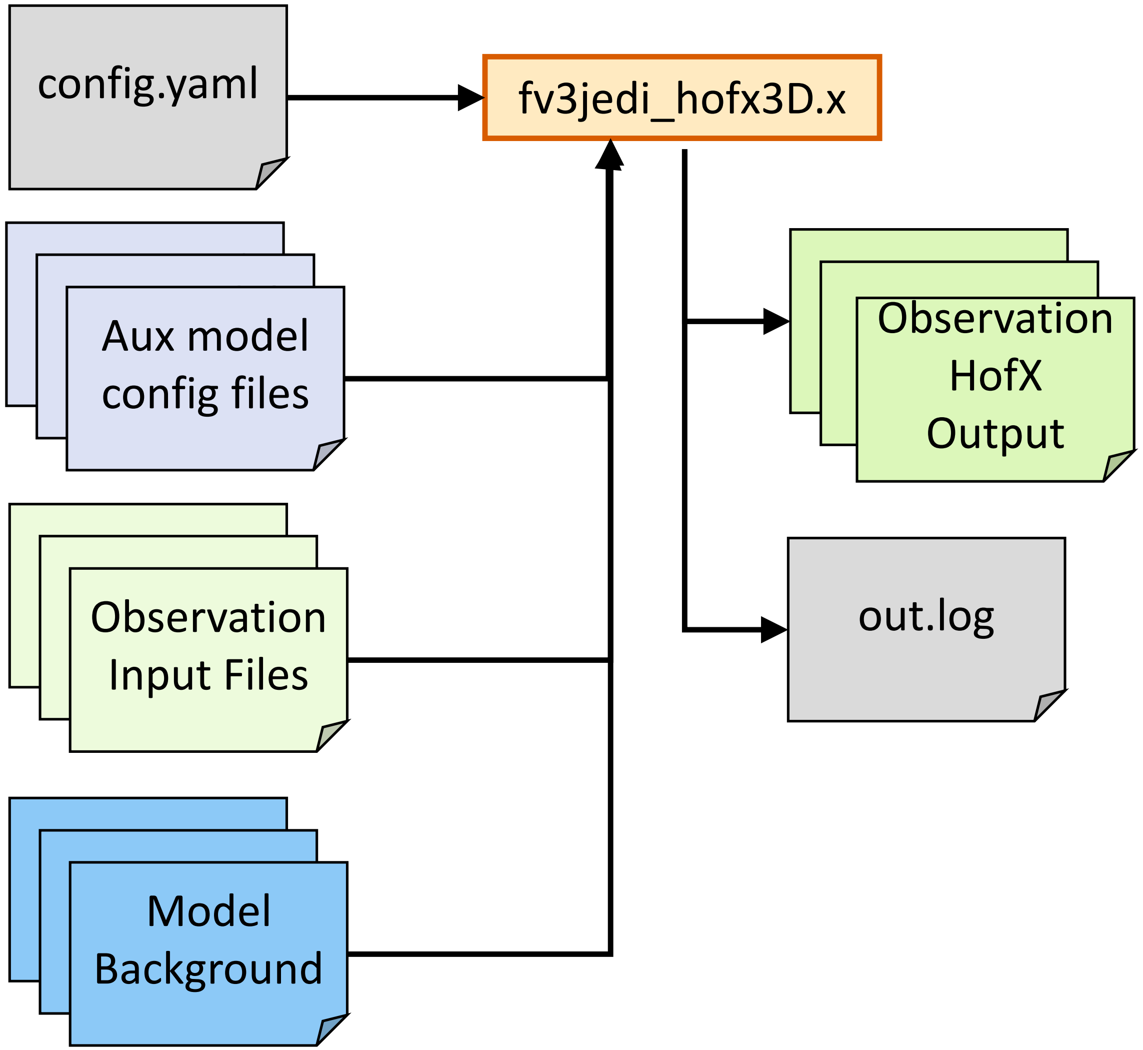


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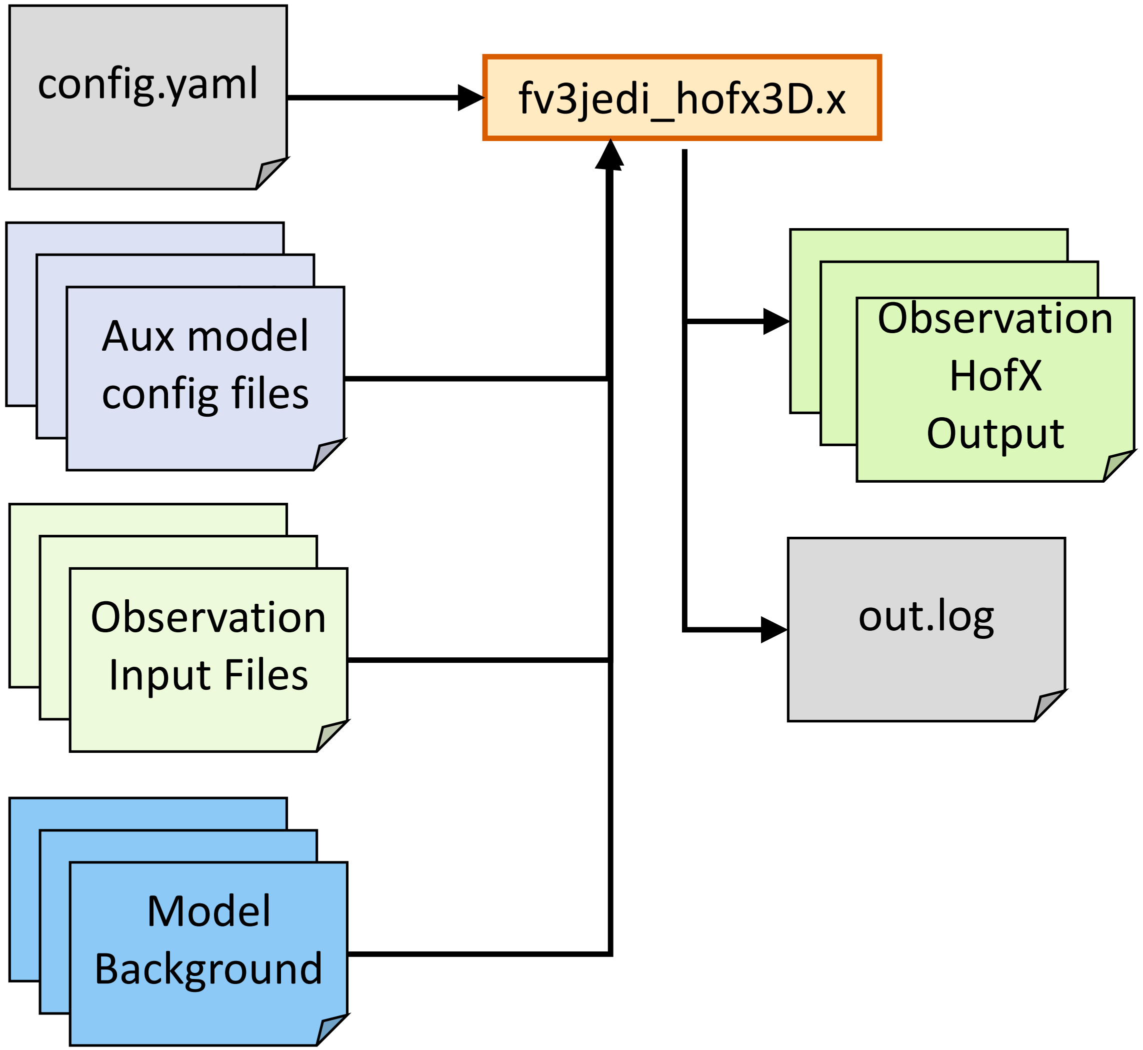


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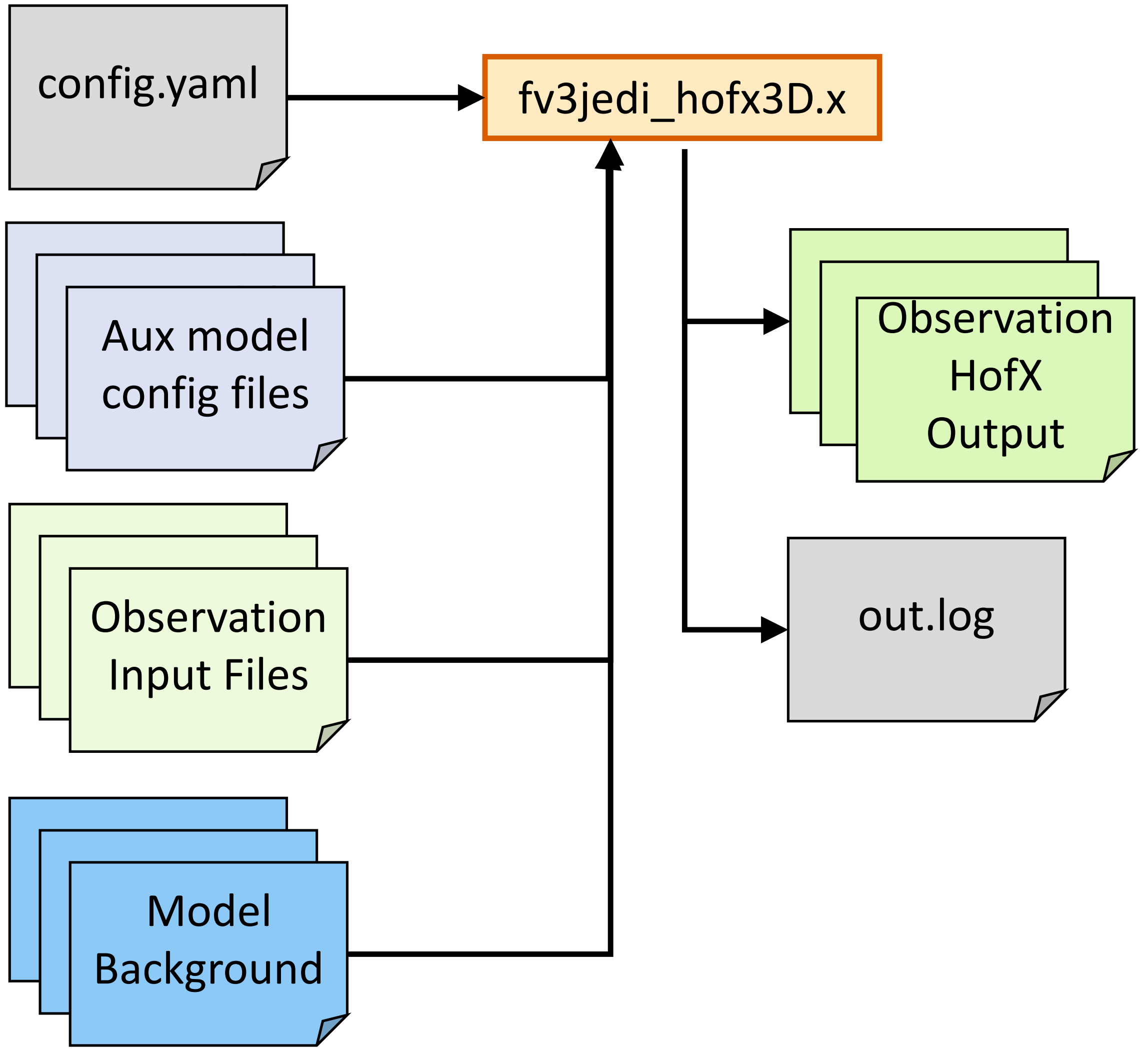


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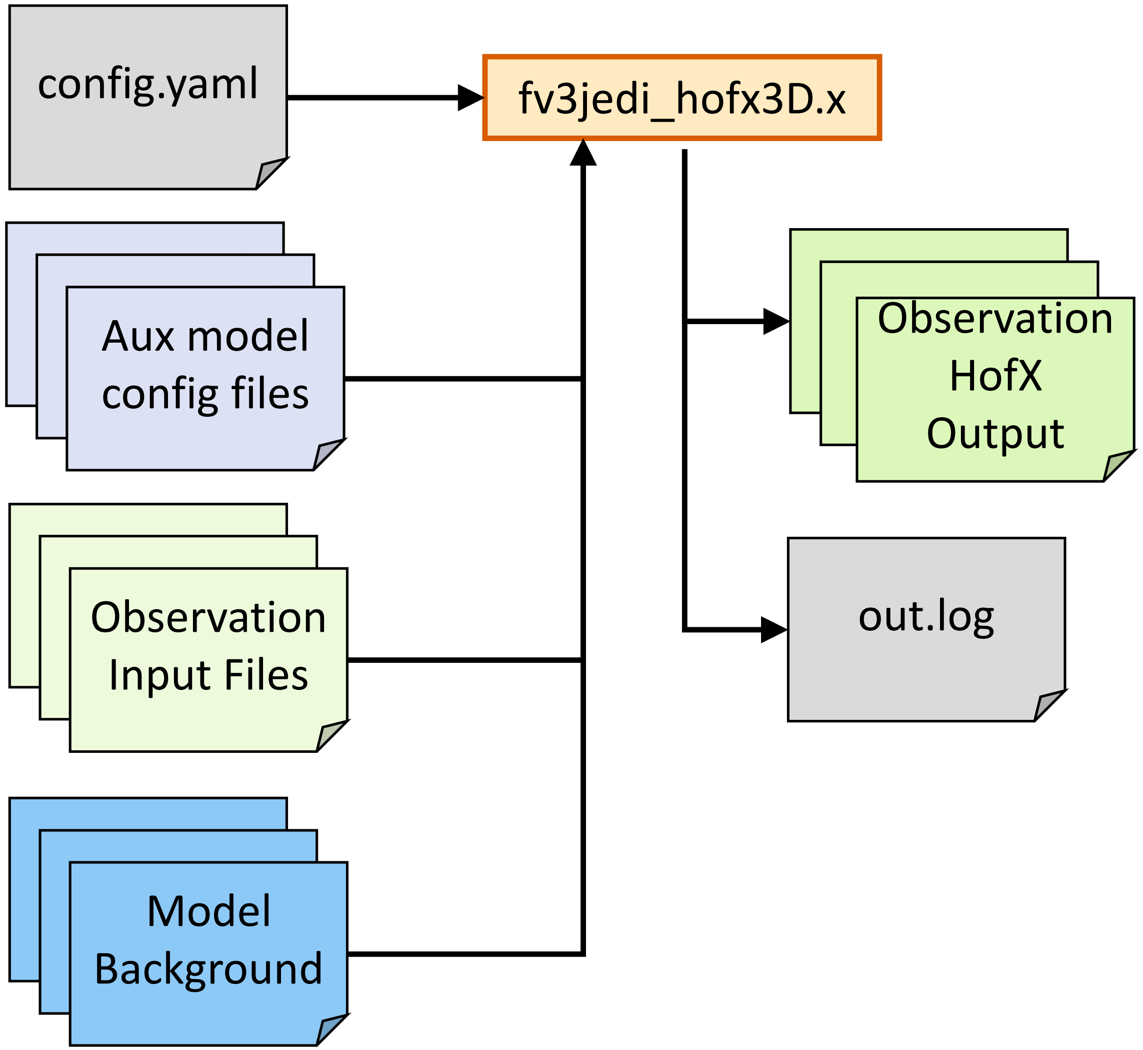


```yaml
nml_file: {{app.config_dir}}/fmsmpp.nml
Assimilation Window:
  Begin: {{window.begin}}
  Length: {{window.length}}
Geometry:
  nml_file: {{app.config_dir}}/input_{{model.desc}}.nml
  trc_file: {{app.config_dir}}/field_table_{{obs.class}}
  pathfile_akbk: {{app.config_dir}}/akbk-{{model.name}}.nc
Initial Condition:
  filetype: {{model.name}}
  datapath_tile: {{app.data_dir}}/{{model.name}}/bg/{{model.date_dir}}
  filename_core: {{model.date_file}}.fv_core.res.nc
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  filename_sfcw: {{model.date_file}}.fv_srf_wnd.res.nc
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  variables: {{model.variables}}
Observations:
  ObsTypes:
  - ObsSpace:
      name: GnssroBndROPP2D
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                  {{model.descr}}_{{obs.desc}}_{{model.date_str}}.nc4"
      simulate:
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    ObsOperator:
      name: GnssroBndROPP2D
      ObsOptions:
Prints:
  frequency: {{app.print_fequency}}
```
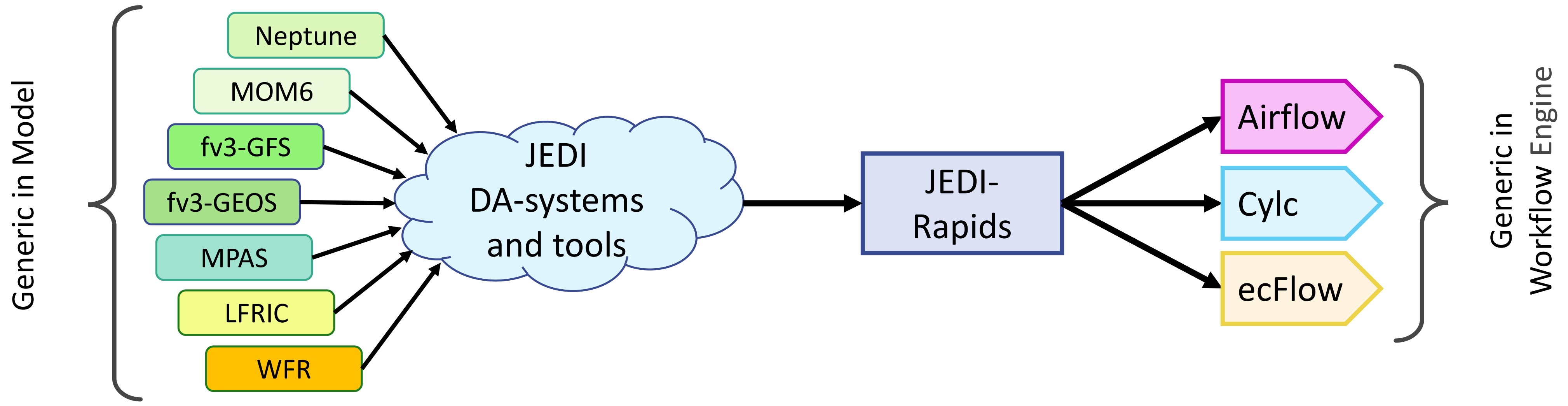

JEDI-Rapids application design goals

- Python 3.6+
- Version controlled repository of
  - Apps (i.e., Tasks, Nodes)
  - Workflows descriptions (i.e., Suites)
- Configuration of Apps YAML / Jinja2
- Generation of JEDI configurations with YAML / Jinja2
- Inheritance and reuse of Apps
- System-agnostic App configurations
- Capture all relevant App state in a single YAML formatted configuration file (Reproducibility)
- Flexibility in workflow system
- Unified dependency and build system for App executables



JEDI Workflow Axes of Generality

Systems
- HPC
  - NOAA; NASA; NCAR;
  - Met Office; NAVY; US DOE
- Cloud (AWS)
- Workstation
- Laptop (Linux, OSX, Win [WSL])

Models
- MPAS
- FV3-GFS / FV3-GEOS
- MOM6 / SOCA
- Neptune
- LFRic
- …

Workflow systems
- ecFlow
- Cylc
- Apache Airflow

Environments
- GNU / Intel / Clang
- OpenMPI / mpich / IMPI / Cray
- Modules / Containers / Native Pkg
- FS: Cloud / Distributed / Parallel

Python vs Shell Scripting for Workflows

Shell Scripts

- Are not portable
  - Dozens of undefined program dependencies.
  - Standard programs can be incompatible across systems
- Lack true debugging facilities
- Are difficult to reuse and compose into larger programs
- Do not provide data structures
- Lack functional and object-oriented language features
- Are dangerously intertwined with environment variables
- Call programs with external state stored in local config files
  - No universal way to capture full state
- Lack native parallelism and threading facilities
- Rely on clunky command line interface to external tools (No APIs)

Python

- Cross-platform
- Dependency management
  - pip, virtualenv, conda, …
- Debuggers
- Profilers
- Advanced Data structures
- Object-oriented and functional programming
- Composable and reusable (Modules)
- RE parsing and string formatting
- Datetime manipulations
- `pathlib` filesystem manipulation
- Logging
- Advanced APIs
- Plotting
- Data format interfaces
- Multiprocessing, threading, futures, …
- Network libraries

JEDI Workflow Features Facilitating Reproducibility

Portability

- Apps are Python-3.6+
- JEDI-stack – Portable environment
  - Provides all library dependencies
  - Lua Modules / Containers
  - Intel / GNU / CLANG
  - OpenMPI / mpich / impi / …

Provenance Tracking

- System information (Python `platform`)
- Software GIT tags/versions
- Input product checksum metadata
- Stored as aux files YAML-format

Data Integrity

- Universal checksums
- S3 ETags
- Storage:
  - DB / AWS S3: Metadata
  - Filesystem: YAML aux files

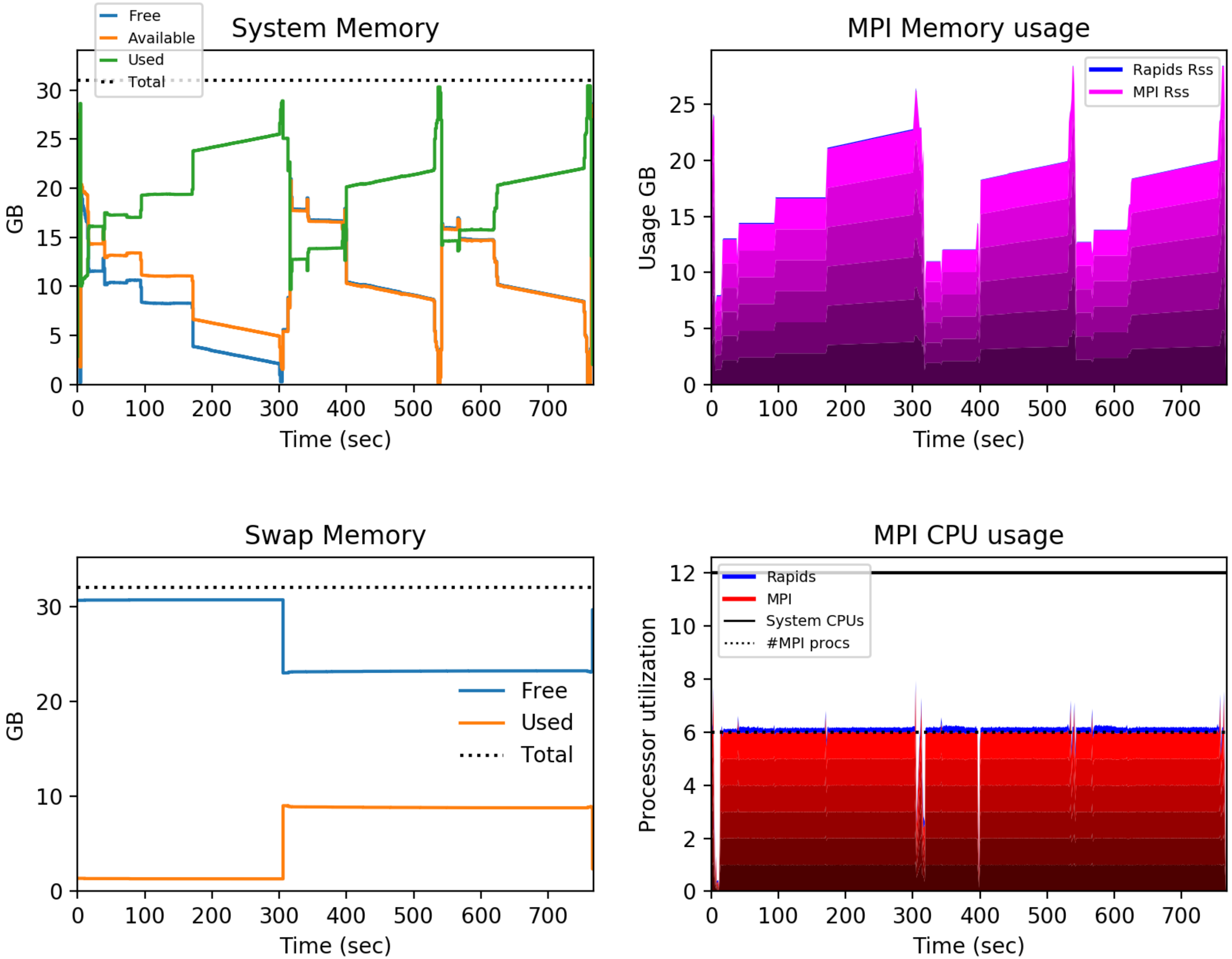
Logging / Configuration

- App YAML Config
  - Python `ruamel` provides round trip preserving of comments
- JEDI Executable config.yaml
- Logs: App / JEDI
- Runtime statistics (CPU / MEM / IO)
  - Python `psutil`

JEDI-Rapids Application Performance Monitoring

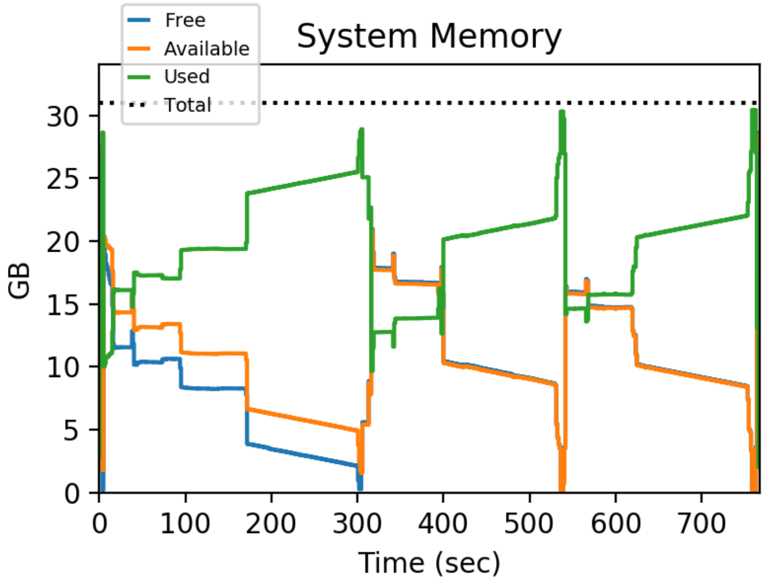
Based on Python `psutil`

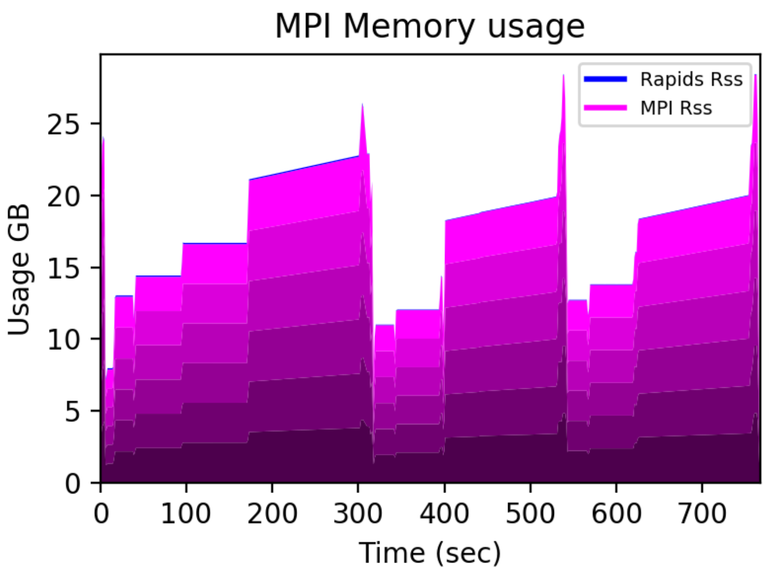
- Cross-platform
- Free, Open-source
- `/proc` filesystem-based
- Highly configurable
  - System memory
  - Swap memory
  - Per-Process memory
    - RSS, PSS, USS
  - System load-avg
  - CPU times (user, system)
  - Threads
  - I/O
  - Context switches
  - System calls
  - Network stats
- JEDI-Rapids polls at regular intervals
  - Saved as Python `pickle`
  - plots are post-processed

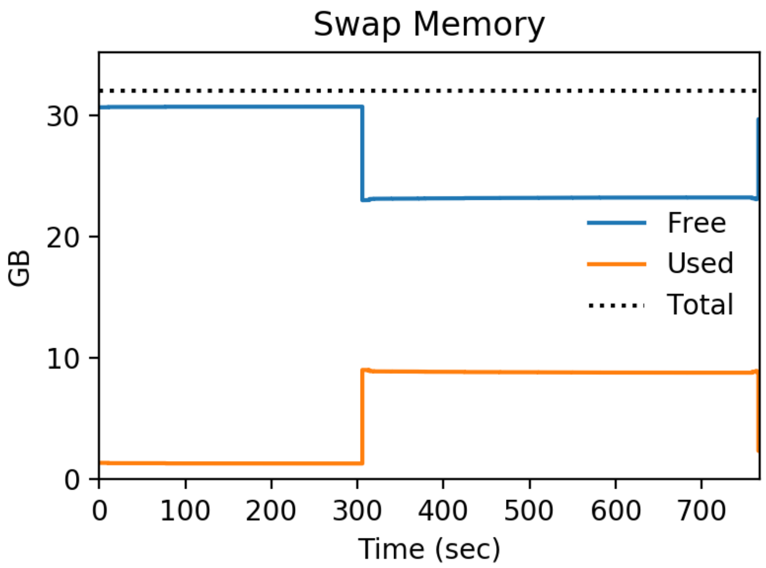


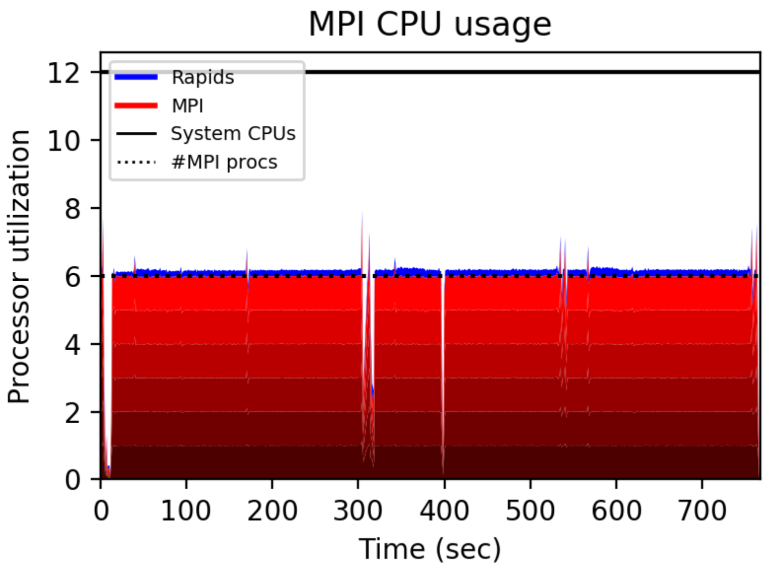
JEDI-Rapids Application Performance Monitoring

- No proprietary software
- No instrumentation of code
- No recompiling or special flags
- Full operational performance
- Works with any language
  - Fortran, C++, Python, etc.
- Works on any system with no special external libraries
- Works on laptops, in the cloud, and on multi-node MPI jobs (aggregation)
- Comparison between runs, machines, problem sizes, algorithms.

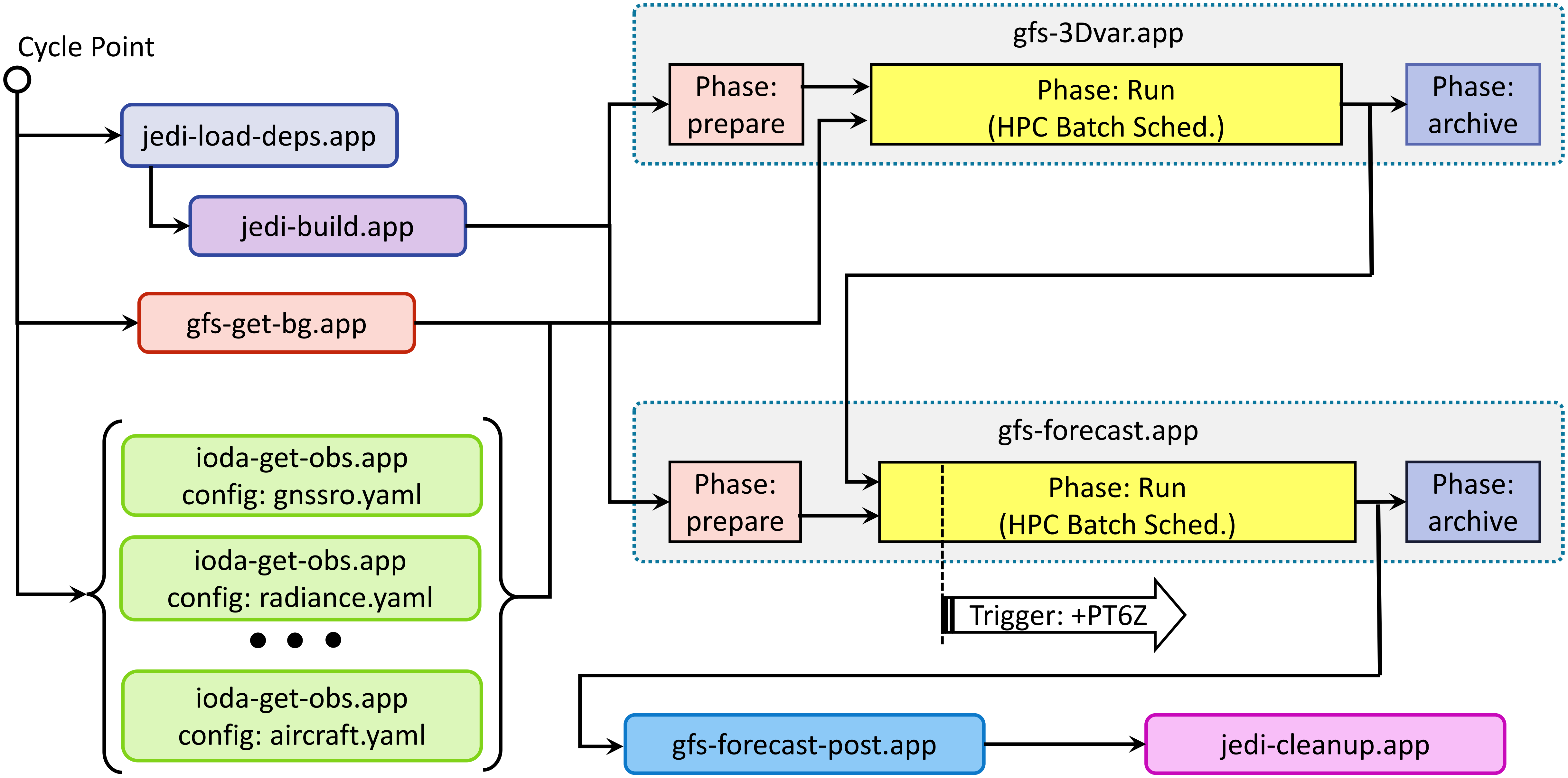




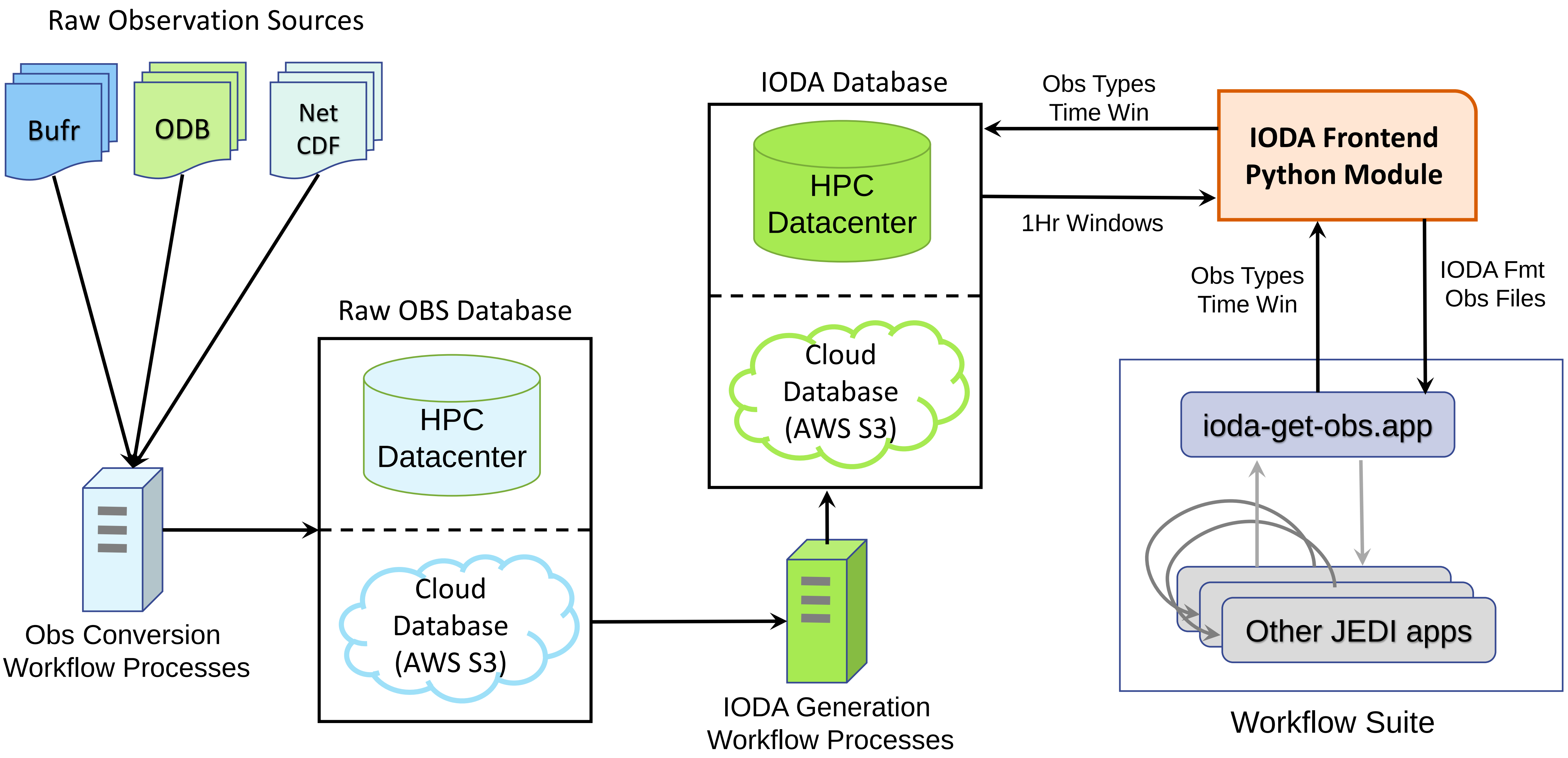




JEDI Example DA Workflow



JEDI IODA Observation Database



JEDI-Rapids Workflow Development Plans

- Automated Workflow Suite Generation
  - Programmatic open-ended cycling DA generic workflows
- Front-end GUI
- Porting to HPC
  - NASA, NOAA, US Navy, US DOE, Met Office
- Universal Observation Ingest System