JEDI in the Cloud

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Virtual Workshop: Weather and Climate in the Cloud ECMWF 8-10 Feb, 2021



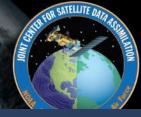








Outline



- I) JEDI Overview
- **II) JEDI Development**
 - **→ Continuous Integration with AWS**
- III) HPC laaS
 - **+ AWS** computing environment
 - **→ JEDI container/cloud benchmarking**
 - **→ JEDI Academies / Training**
- IV) Web Applications
 - **→ NRT Observation monitoring**
- V) Summary and Outlook
 - + Broader JCSDA context

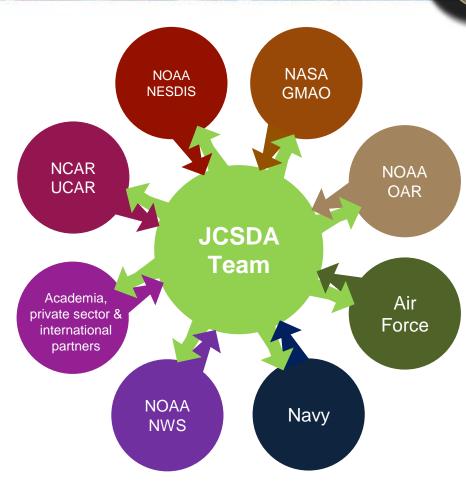


Joint Center for Satellite Data Assimilation



JCSDA

A multi-agency research center created to improve the use of satellite data for analyzing and predicting the weather, the ocean, the climate and the environment.



WHO

Distributed staff

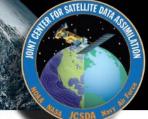
HOW

Joint operating plan

WHAT

Critical path to operations

JEDI



FV3 (GFS+GEOS) (NOAA/NASA)

> MPAS (NCAR)

UM & LFRic (UKMO)

> SOCA (JCSDA)

Toy models (Lorenz 95, QG, shallow water)

...

Joint Effort for Data assimilation Integration

JEDI

First Release Oct, 2020

A Next-Generation
Unified
DA System

Radiosondes

Radiance

Aircraft

Aerosols

GNSSRO

...

JEDI

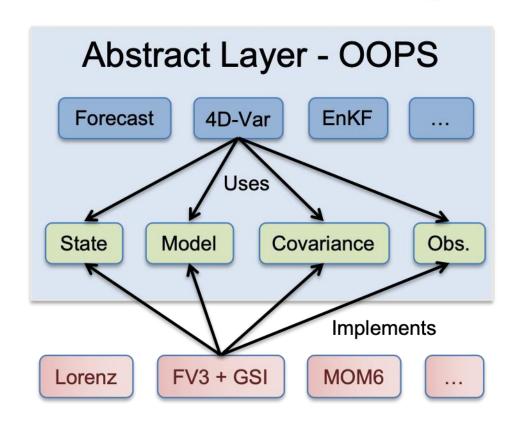


Motivations

- Reduce duplication of effort among partners
 - New obs, DA algorithms
- Unified
 - same DA algorithms for atmosphere, ocean, coupled & toy models
- + Promote R2O/O2R

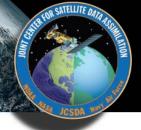
Approach

- ◆ Exploit object-oriented & generic programming
- **→** Separation of concerns
- → Agile, collaborative development environment



- C++ (high-level)
- Fortran (low-level)

II: JEDI Development: CI with AWS



Each PR tested with multiple

compiler/mpi combinations

- GNU / OpenMPI
- Clang / MPICH
- Intel / IMPI





- AWS CodeBuild:
 - scales easily with computational needs
 - run multiple configurations in parallel using containers

Reviewers

Code
developer

Pull Request

Reviewers

Merge Code

Web hooks trigger
Cl pipelines, sync
private & public
repos, enforce
branch naming
conventions

CI also checks code coverage

AWS CodePipeline for comprehensive downstream testing of dependent repos



Higher-tier application-level testing to be handled through nightly/weekly cron jobs

III: HPC laaS



Single Development node

- **→** For development, optimization
- → Easy to use launch script
- **→** Can terminate/stop from EC2 console
- Custom AMI
- **→** gnu-openmpi, intel-impi environment modules
- → Docker, Singularity, Charliecloud



```
18:34 $ jedinode.py --help
Usage: jedinode.py [OPTIONS]
Options:
                                  [required]
  --key TEXT
                        ssh key
  --type TEXT
                        Instance type (default c5.4xlarge)
  --ncores INTEGER
                        Number of cores (you can omit this for most instance
                        types)
  --securitygroup TEXT Security group id (default is virginia-default)
                        Region (default is us-east-1)
  --region TEXT
  --spot
                        spot market (default is False)
                        Max Price (defaults to on-demand price; only used if
  --maxprice TEXT
                        spot is set)
  -h. --help
                        Show this message and exit.
```

III: HPC laaS



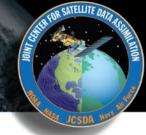
ParallelCluster

- → For applications, optimization, testing
- → Autoscaling: cluster size adjusts on demand
- **→** EFS, FSx for lustre
- ◆ Intel 19 compilers/mpi
- **→** gnu-openmpi, intel-impi stacks
- ♦ AWS-provided AMI; security patches, latest hardware support
- **→ Post-install script: Singularity, git-lfs...**
- → Spot pricing or on demand
- ◆ VPC (public master, private compute nodes) with subnets in us-east-1c (best availablity)
- → Dynamic placement group for collocated resources

Unified approach to facilitate maintenance:

Intel compilers and environment modules (gnu-openmpi, intel-impi) provided by means of an external volume that is auto-mounted at boot time

Supercontainers



JEDI cloud applications can be built and run either with environment modules or with software containers

Container benefits

- Portability
- Reproducibility
 - Version control (git)
- Bring your own environment
- Efficiency / workflow
 - Develop on laptops, run on HPC/cloud
 - Get new users up and running quickly

JEDI Supercontainers

- Singularity
 - Development containers
 - Application containers (multi-stage build with intel runtime libraries)
- Enhanced components
 - Infiniband drivers
 - PMI
 - UCX, KNEM, XPMEM



Container/Cloud Benchmarking



Benchmark FV3-GFS JEDI 3DVar Application

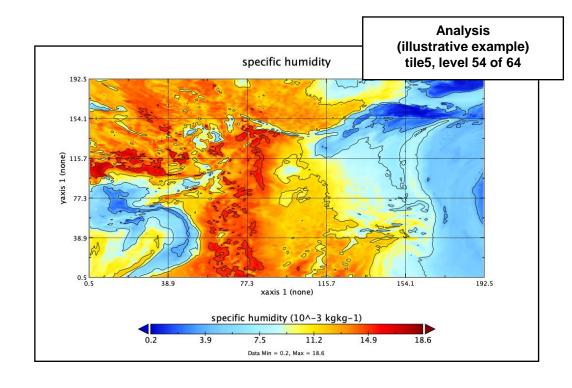
- Resolution c192
- ~9 of 12 million obs pass QC
- Inner loop: 30 iterations
- Outer loop: 2 iterations
- 864 MPI tasks (12x12x6)

~12 million obs

Aircraft, Radiosonde, Rass, Satwind, Scatwind, Vadwind, AMSUA-NOAA19, AIRS-AQUA, IASI-METOPA, CRISFSR-NPP

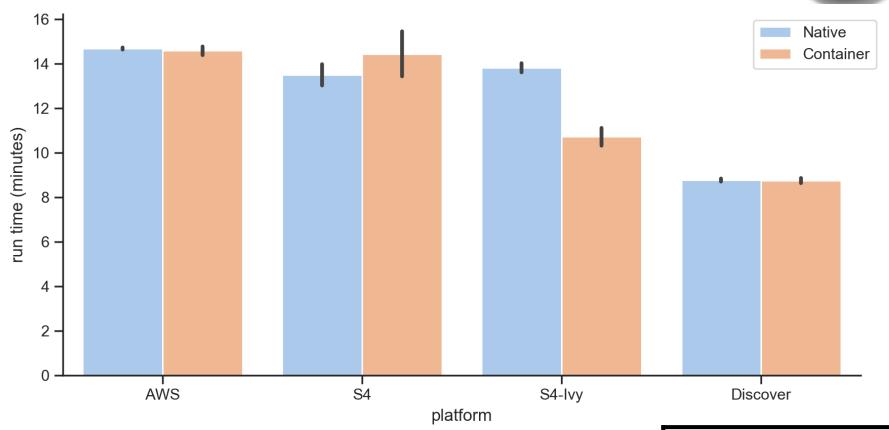
Platforms

- Discover: NASA NCCS
- S4: SSEC/Univ. Wisconsin
- AWS
 - 24 c5n.18xlarge nodes
 - 36 cores/node
 - Elastic Fabric Adapter (EFA)



Container/Clloud Benchmarking





No overhead for running in the container

Estimated AWS cost	
On demand	\$23
Spot	\$7

Container/Cloud Benchmarking



Performance Tuning on AWS

Mean run time on previous slide for AWS cluster: 14.59 min inside container, 14.69 min outside container

- ~ 20 sec: FSx for Lustre instead of EBS
- ~ 70 sec: MPI tuning
- ~ 150 sec: mitigate memory fragmentation due to VM caching (sudo echo 3 > /proc/sys/vm/drop_caches)

Now running about:

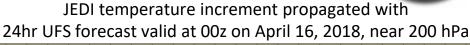
~ 10.6 min outside container

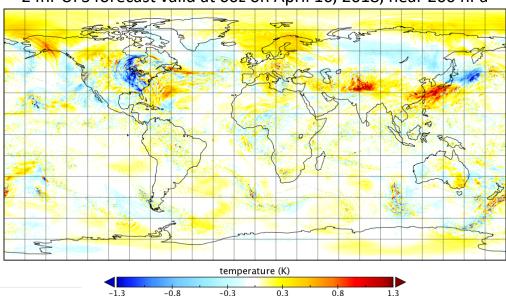
May be possible to get it under 10 min Recall Discover ~ 8.8 min

Forecast Model Benchmarking

Ton Marie Trans

- UFS (pre-)operational C768 (13km) global configuration
- 10-day forecast with NEMSfv3gfs on 48 AWS c5.x18large nodes
 - 36 cores, 144GB mem, 25GB/s network, Intel 19 with iMPI
 - 1728 cores in total
- model run takes 7 min 22s real time per simulated day



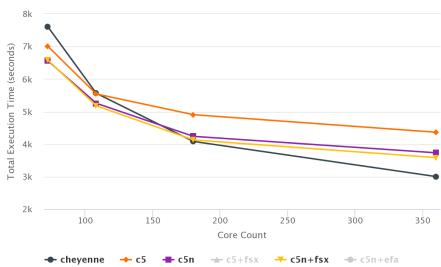


Operational GFS v15

Data Min = -4.5, Max = 3.7, Mean = 0.0

Results prior to EFA (Early 2019)

WRF Performance on AWS (vs. Cheyenne)



JEDI Training

CSDA WATER

JEDI Academy

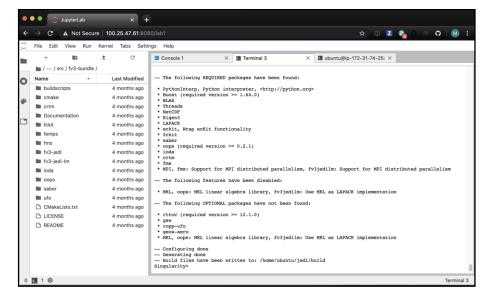
- Biannual (disrupted by COVID)
- 4-5 days each, varying locations
- ~40 participants
- Mix of lectures and practicals
- Virtual in Nov-Dec 2020

Activities use AWS

- Participants divided into 20-40 groups, each with their own AWS EC2 instance
- EC2 instances accessed via JupyterLab web interface
- Groups pull singularity container and build, run JEDI applications
- Estimated cost ~ \$100/day



Jupyterlab interface includes one or more ssh consoles, a python interpreter, a navigation panel, and an image viewer



Self-paced online tutorials also made available through a jcsda-tutorial public AMI and containers https://jedi-docs.jcsda.org/en/latest/learning/tutorials/

IV) NRT Observation Monitoring





JCSDA Near-Real-Time Observation Monitoring

http://nrt.jcsda.org

NOAA GFS

Resolution: c768

6-hr Assimilation Window Begins: 2021-02-02T15:00:00

Application Goals

This is a near real-time demonstration of the JEDI H(X) application, which simulates observations from a forecast model background state in correspondence with actual observations.

Configuration

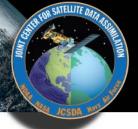
Observations are processed in 6-hr windows beginning at 0300Z, 0900Z, 1500Z, and 2100Z. Analysis is generated every 6 hours with an approximately 72 hour delay due to GFS.

Background Information

Computing H(X) is the first step in assimilating observation data into a forecast system. JEDI supports the end-to-end process of data assimilation, through unified forward operators (UFO), an interface for observation data access (IODA), variational solvers from

Testbed for development & validation of observation operators

NRT Observation Monitoring



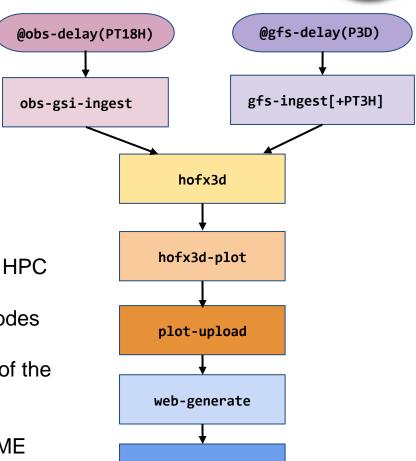


JEDI NRT Unified Workflow



```
cylc-monitor 1d83305c-50b4-4cf0-ac2b-9c425ee8effc
runaheadwaitingheldnumusexpiredreadysubmit-failedsubmit-retryingsubmittedretryingrunningfailedsucceeded
updated: 2020-05-05718:59:08Z
state summary: 5 1 6 15

20200501T1500Z web-publish
20200501T1500Z web-publish
20200501T1500Z ingest hofx3d plot plot-upload web-generate web-publish
20200502T0300Z obs-ingest hofx3d plot plot-upload
20200502T1090Z obs-ingest hofx3d plot plot-upload
20200502T1090Z obs-ingest hofx3d plot
20200502T1090Z obs-ingest hofx3d plot
20200502T100Z obs-ingest hofx3d
20200502T100Z obs-ingest hofx3d
20200503T1000Z gfs-ingest
20200503T1000Z gfs-ingest
20200503T1000Z gfs-ingest
20200503T1000Z gfs-ingest
20200503T1000Z obs-ingest
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20200503T100Z obs-ingest
20200503T00Z obs-ingest
20200503T00Z obs-ingest
```



web-publish

- JCSDA workflow software is portable across HPC and Cloud resources.
- Rapidly initialize and deploy EC2 compute nodes based on prepared AMI images.
- Depending on resource costs different parts of the workflow can be run on different machine instances.
- Data is moved from S3 to EBS and local NVME storage depending on access requirements and machine resources

V: Summary & Outlook



JEDI Cloud Computing

- → CI / development
- **→ HPC laaS: JEDI Applications, optimization**
- **→ JEDI Training: Academies, Tutorials**
- https://nrt.jcsda.org NRT H(x)















JCSDA

- → More web Apps
 - Observation Impact: https://ios.jcsda.org
 (serverless FSOI diagnostics on-demand)
 - **⊙NRT Marine DA:** https://soca.jcsda.org
- + R2D2
 - Research Repository for Data & Diagnostics
- → Machine Learning















