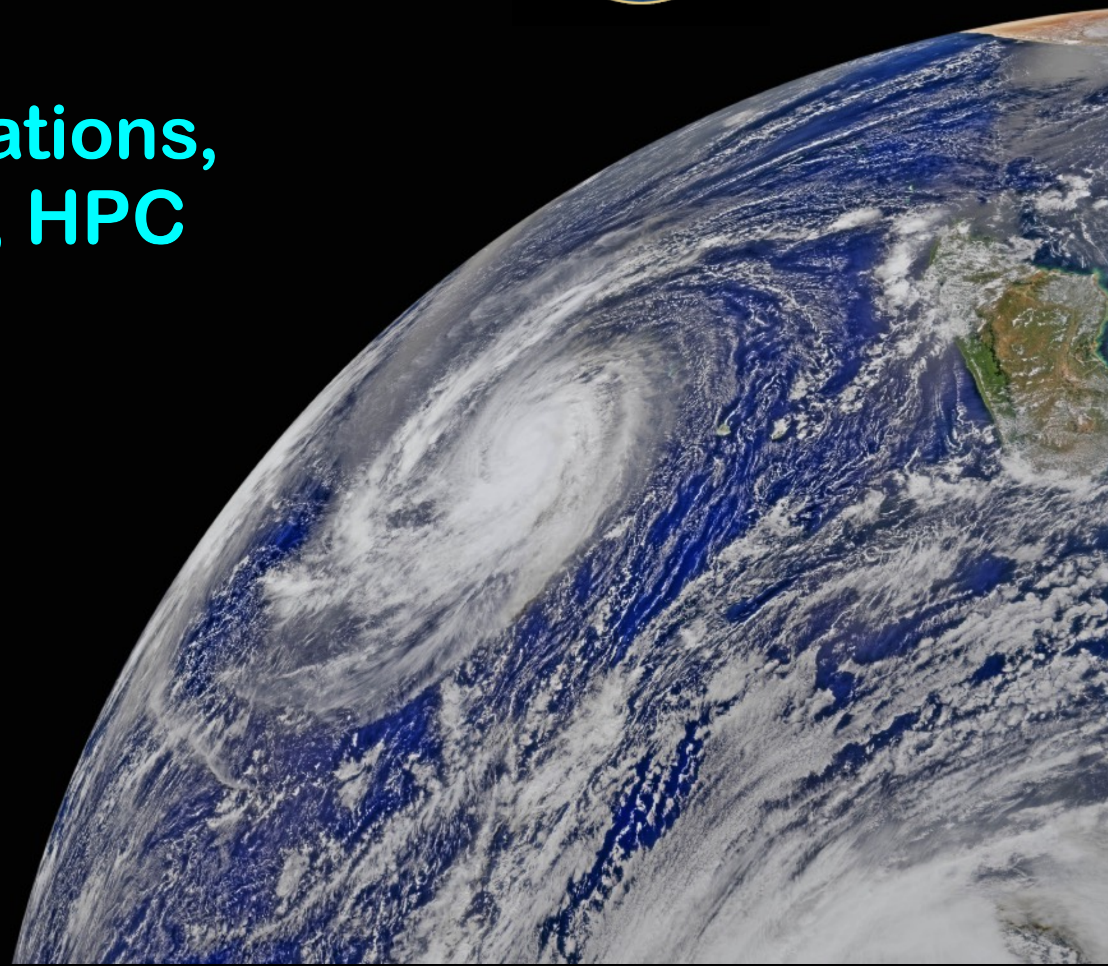
Accessing, Building and Running JEDI

Laptops, Workstations, Clusters, Cloud, HPC



Outline

I) Acquire dependencies

- ✦ JEDI Portability overview
- ✦ Software containers
- ✦ HPC environment modules
- ✦ Cloud

II) Build JEDI

- ✦ JEDI bundles
- ✦ CMake, ecbuild

Note: in today's practicals you will not need to build JEDI - you will only run it. But, knowing how to access, build, and run JEDI may help you *after* today

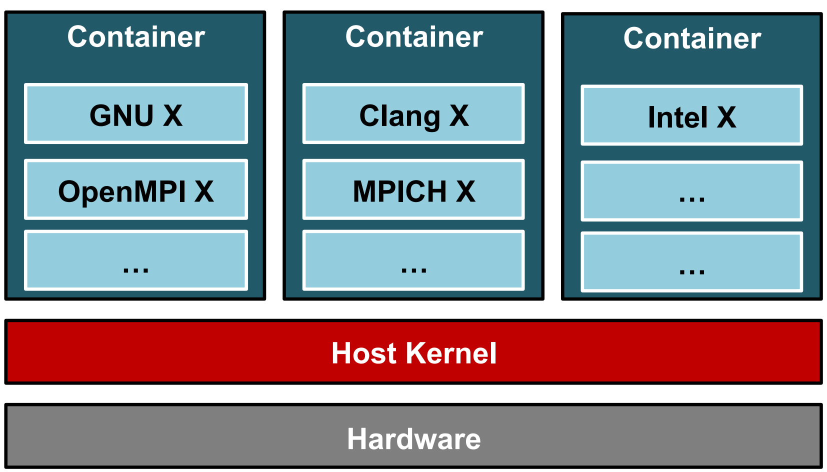
How can I Run JEDI?

- **Application container**
  - ✦ A software container that includes JEDI and all it’s dependencies, ready to run
- **Development container**
  - ✦ Includes JEDI dependencies - you download and build JEDI yourself
- **Pre-Made Environment Modules**
  - ✦ JEDI dependencies available on Hera, Orion, Discover, S4, Cheyenne, Gaffney, and the Amazon cloud (through AMIs)
  - ✦ You download and build JEDI yourself
- **Build your own Environment Modules**
  - ✦ Jedi-stack build system: https://github.com/JCSDA/jedi-stack
  - ✦ You build JEDI and all of its dependencies

What is a container?

Software container (working definition)

A packaged user environment that can be "unpacked" and used across different systems, from laptops to cloud to HPC



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 Software Dependencies

- Essential
  - ✦ Compilers, MPI
  - ✦ CMake
  - ✦ SZIP, ZLIB
  - ✦ LAPACK / MKL, Eigen 3
  - ✦ NetCDF4, HDF5
  - ✦ udunits
  - ✦ Boost (headers only)
  - ✦ ecbuild, eckit, fckit
  - ✦ bufr
- Useful
  - ✦ PNETCDF
  - ✦ Parallel IO
  - ✦ nccmp, NCO
  - ✦ Python tools (netcdf4, matplotlib, cartopy…)
  - ✦ json-schema-validator

What do the containers and modules contain?

Common versions among users and developers minimize stack-related debugging

Environment Modules

Example: Discover (NCCS)

```
(base) mmiesch@discover34:~> module purge
(base) mmiesch@discover34:~> module load jedi/intel-impi
(base) mmiesch@discover34:~> module list

Currently Loaded Modules:
  1) git/2.24.0                 9) udunits/2.2.26         17) eigen/3.3.7
  2) git-lfs/2.10.0            10) mpi/impi/19.1.0.166    18) bufrlib/11.3.2
  3) jedi-python/3.8.3         11) jedi-impi/19.1.0.166   19) cmake/3.17.0
  4) comp/gcc/9.2.0            12) hdf5/1.12.0            20) ecbuild/jcsda-3.3.2.jcsda3
  5) comp/intel/19.1.0.166     13) pnetcdf/1.12.1         21) eckit/jcsda-1.11.6.jcsda2
  6) jedi-intel/19.1.0.166     14) netcdf/4.7.4           22) nco/4.7.9
  7) szip/2.1.1                15) nccmp/1.8.7.0          23) pio/2.5.1-debug
  8) zlib/1.2.11               16) boost-headers/1.68.0   24) jedi/intel-impi/19.1.0.166-v0.4
```

jedi-stack leverages native compilers and mpi libraries

Other stack components are built from these

Container Technologies

- ## Docker
  - Main Advantages: industry standard, widely supported, runs on native Mac/Windows OS
  - Main Disadvantange: Security (root privileges)

- ## Singularity
  - Main Advantages: Reproducibility, HPC support
  - Main Disadvantage: Not available on all HPC systems
  - Preferred platform for scientific applications

JCSDA provides a public ubuntu 18.04 AMI that comes with Singularity, Charliecloud, and Docker pre-installed

Current containers

- **Development**
  - gnu-openmpi-dev (D, S, C)
  - clang-mpich-dev (D, S, C)
  - intel-oneapi-dev (DIY)

Distribution

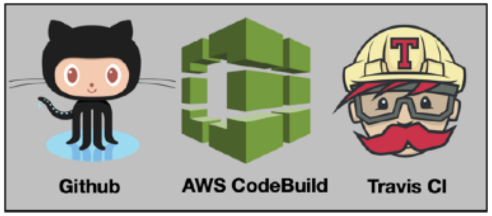
Docker Hub
Sylabs cloud
AWS S3 (public)

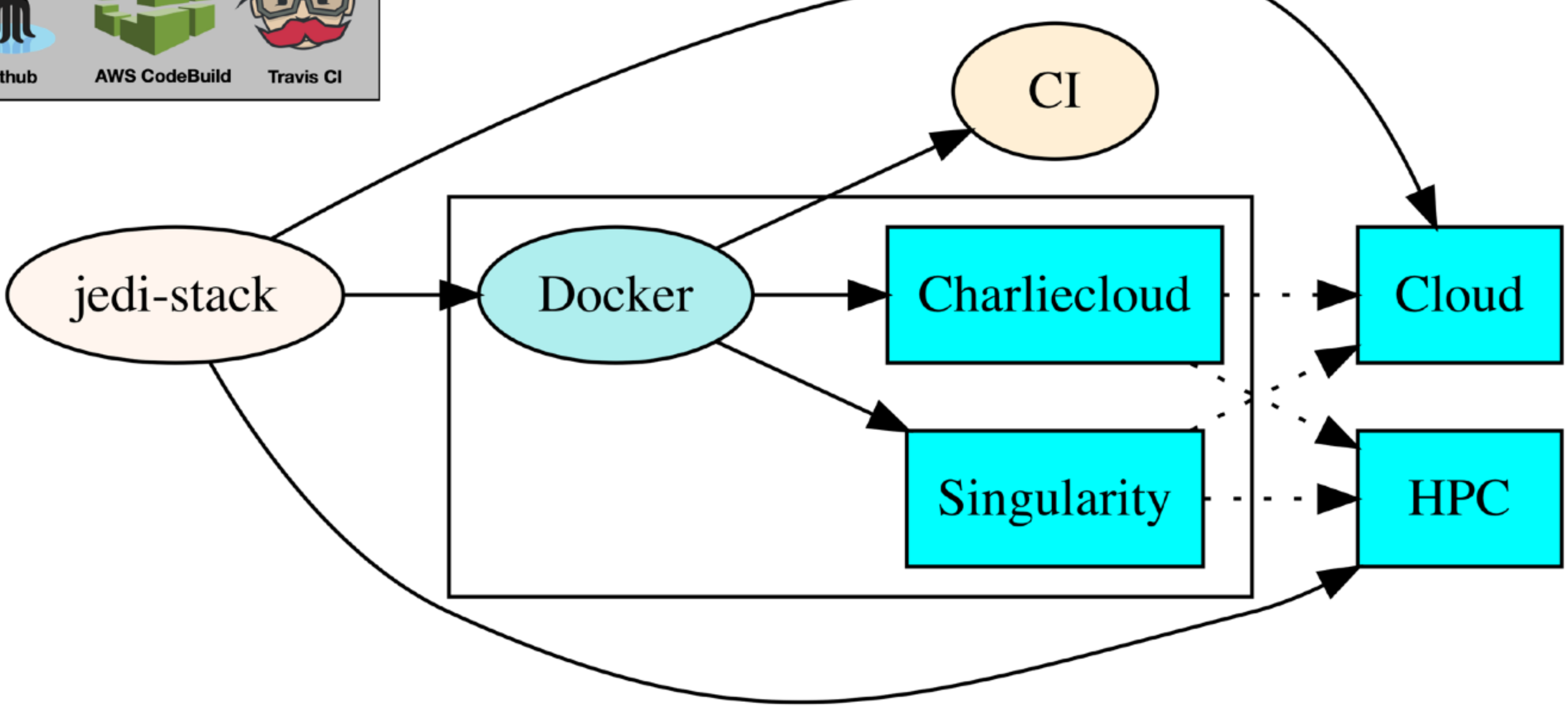
- **Application**
  - Tutorial (S)
  - intel 19 and 2021 One API (S)

```
singularity pull library://jcsda/public/jedi-gnu-openmpi-dev
singularity shell -e jedi-gnu-openmpi_latest.sif
```

http://data.jcsda.org/pages/containers.html

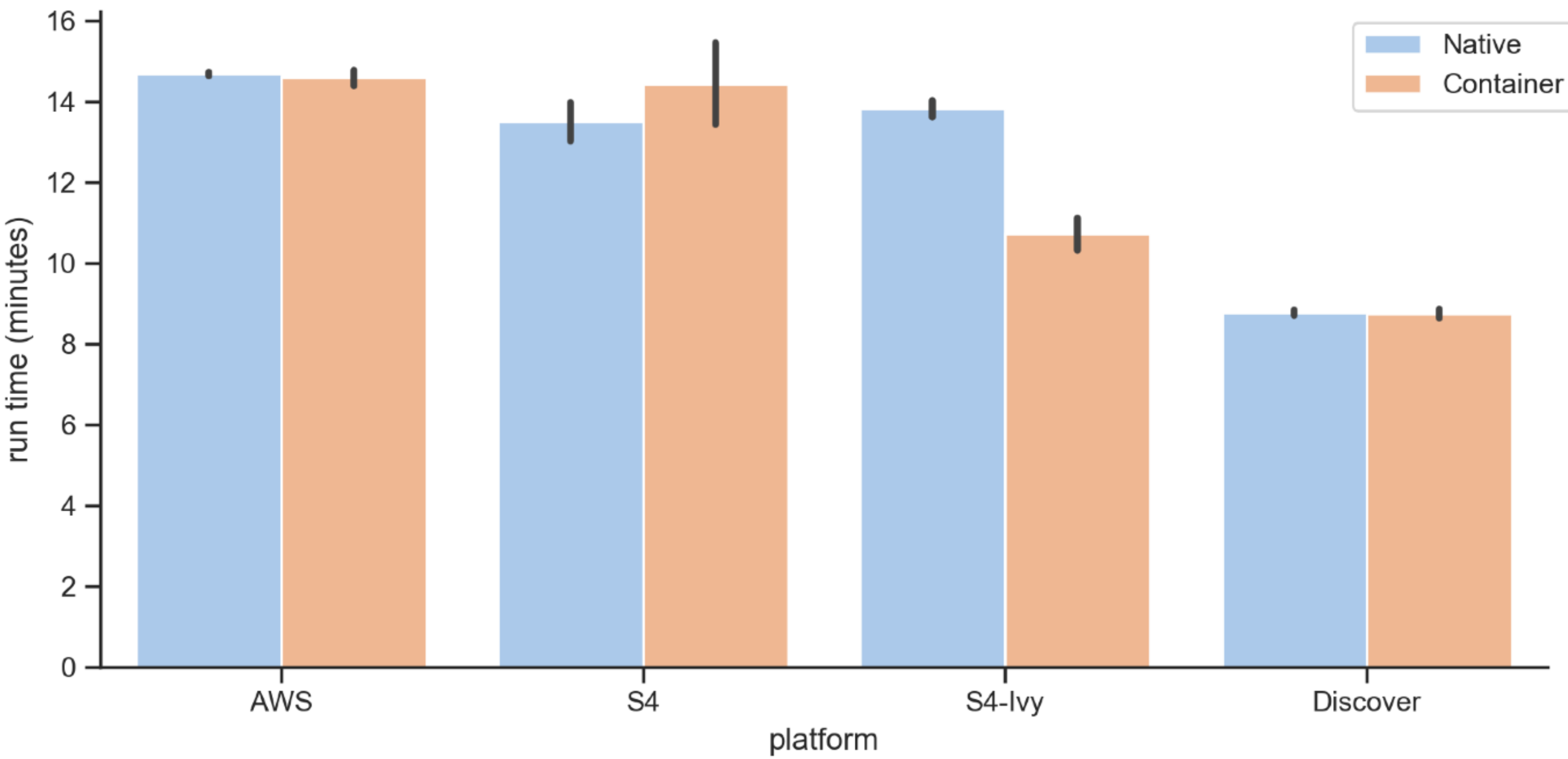
Unified Build System





Tagged jedi-stack releases can be used to build tagged containers, AMIs, and HPC environment modules, ensuring common software environments across platforms

Supercontainers!



With a little care, containers can be run across nodes on HPC systems with no overhead

JEDI 3DVar Application

864 MPI tasks, 12M observations
FV3-gfs c192

II: JEDI Build System

The JEDI is code organized into bundles that identify all the GitHub repositories necessary to build and run the applications

CMake build system: ecbuild = CMake macro package developed and maintained by ECMWF

CMakeLists.txt file for fv3-bundle

```
# Create project
project( fv3-bundle VERSION 1.0.0 LANGUAGES C CXX Fortran )

[...]

# External (required) observation operators
ecbuild_bundle( PROJECT crtm GIT "https://github.com/jcsda/crtm.git"   TAG v2.3-jedi )

# Core JEDI repositories
ecbuild_bundle( PROJECT oops  GIT "https://github.com/jcsda/oops.git"  BRANCH develop UPDATE )
ecbuild_bundle( PROJECT saber GIT "https://github.com/jcsda/saber.git" BRANCH develop UPDATE )
ecbuild_bundle( PROJECT ioda  GIT "https://github.com/jcsda/ioda.git"  BRANCH develop UPDATE )
ecbuild_bundle( PROJECT ufo   GIT "https://github.com/jcsda/ufo.git"   BRANCH develop UPDATE )

# FMS and FV3 dynamical core
ecbuild_bundle( PROJECT fms GIT "https://github.com/jcsda/FMS.git"                          TAG 1.0.0.jcsda )
ecbuild_bundle( PROJECT fv3 GIT "https://github.com/jcsda/GFDL_atmos_cubed_sphere.git" TAG 1.0.0.jcsda )

# fv3-jedi and associated repositories
ecbuild_bundle( PROJECT femps       GIT "https://github.com/jcsda/femps.git"                 BRANCH develop UPDATE )
ecbuild_bundle( PROJECT fv3-jedi-lm GIT "https://github.com/jcsda/fv3-jedi-linearmodel.git" BRANCH develop UPDATE )
ecbuild_bundle( PROJECT fv3-jedi    GIT "https://github.com/jcsda/fv3-jedi.git"              BRANCH develop UPDATE )
```

Building a Bundle

```
git clone https://github.com/JCSDA/fv3-bundle.git    1
mkdir build                                          2
cd build
ecbuild ../fv3-bundle                                3
make update                                          4
make -j4                                             5
ctest                                                6
```

1. Download the bundle repository from GitHub
2. Create a build directory
3. Run ecbuild (CMake) to generate a build system
4. Pull the latest source code from GitHub
5. Compile
6. Run the test suite for the bundle

Running a JEDI Application

Each application just takes a single configuration file as input, in yaml format

```
# Define JEDI bin directory where the executables are found
# ----------------------------------------------------------
export jedibin=$HOME/jedi/build/bin

# Run the BUMP parameter scripts to produce the B matrix
# ------------------------------------------------------
mpirun -np 6 $jedibin/fv3jedi_parameters.x config/bumpparameters_nicas_gfs.yaml

# Run the variational application
# -------------------------------
mpirun -np 18 $jedibin/fv3jedi_var.x config/4denvar.yaml

# Compute the increment for plotting
# ----------------------------------
mpirun -np 6 $jedibin/fv3jedi_diffstates.x config/4denvar-increment.yaml
```

A JEDI Configuration file


```yaml
cost function:
  cost type: 4D-Ens-Var
  analysis variables: [ua,va,T,ps,sphum,ice_wat,liq_wat,o3mr]
  window begin: '2018-04-14T21:00:00Z'
  window length: PT6H
  subwindow: PT3H
  background:
    states:
    - filetype: gfs
      datapath: /opt/jedi/build/fv3-jedi/test/Data/inputs/gfs_c12/bkg/
      filename_core: 20180414.210000.fv_core.res.nc
      filename_trcr: 20180414.210000.fv_tracer.res.nc
      filename_sfcd: 20180414.210000.sfc_data.nc
      filename_sfcw: 20180414.210000.fv_srf_wnd.res.nc
      filename_cplr: 20180414.210000.coupler.res
      state variables: [ua,va,T,ps,sphum,ice_wat,liq_wat,o3mr,phis,
                        slmsk,sheleg,tsea,vtype,stype,vfrac,stc,smc,snwdph,
                        u_srf,v_srf,f10m]
# [...]
observations:
  - obs space:
      name: AMSUA-NOAA19
      obsdatain:
        obsfile: /opt/jedi/build/fv3-jedi/test/Data/obs/testinput_tier_1/amsua_n19_obs_2018041500_m.nc4
      simulated variables: [brightness_temperature]
      channels: 10
    obs operator:
      name: CRTM
      Absorbers: [H2O,O3]
      obs options:
        Sensor_ID: amsua_n19
```


A taste of what a [JEDI configuration file](#) looks like

(you'll see more in the other lectures and activities)

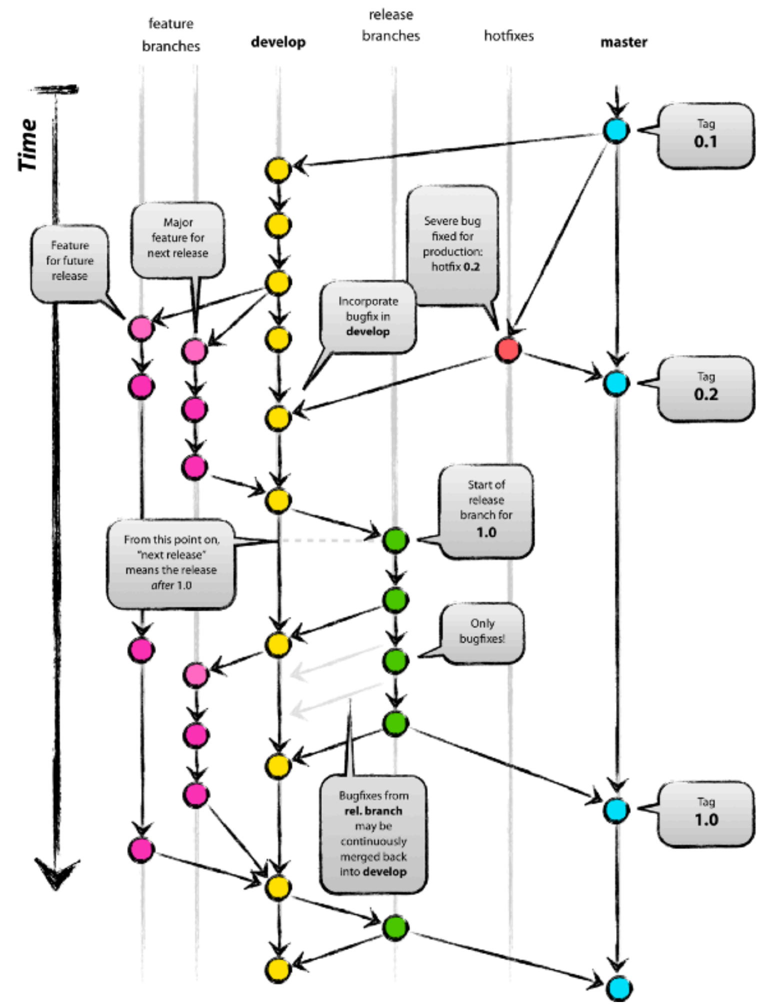
Contributing to JEDI

Source code

https://github.com/JCSDA

Code Contributions handled via Pull Requests

- ✦ Work from forks
- ✦ Use git-flow branch naming conventions
- ✦ Document and test your code
- ✦ Expect Code reviews, CI testing

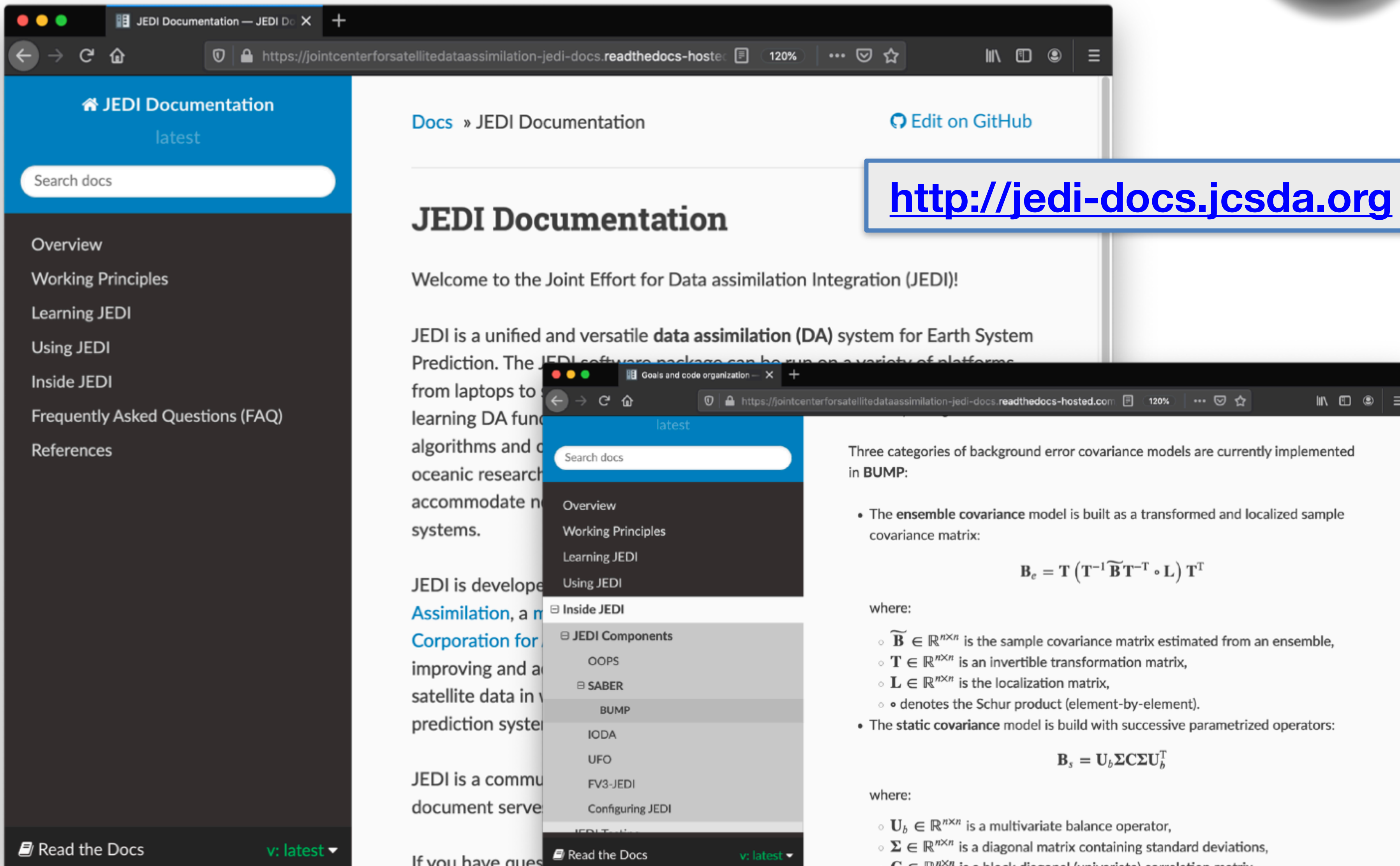


User/Developer forums

https://forums.jcsda.org

https://nvie.com/posts/a-successful-git-branching-model/

JEDI User/Developer Manual



http://jedi-docs.jcsda.org


Questions Welcome