CROW: Python-based Configuration Toolbox for Operational and Development Workflows

CROW Review April 28th 2020

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Outline

- Purpose of CROW What problem are we solving?
- High-level overview of CROW design and use example with global-workflow/FV3GFS
- Development of CROW
- Implementations of CROW
- What will community support for CROW look like?

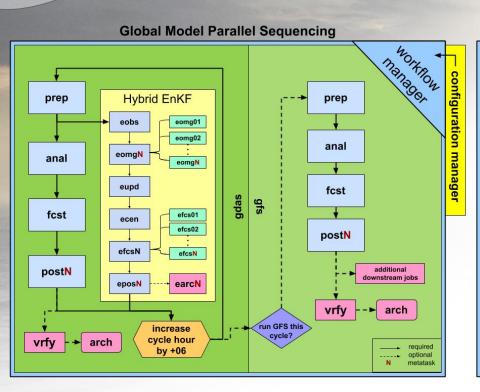
Problem statement

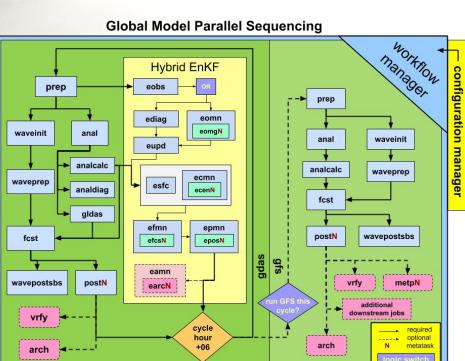
Increasing complexity of operational and developmental workflows poses significant challenges for configuration.

Has become difficult to:

- Ensure consistency and quality in configuration
- Document and archive configuration settings (e.g. provenance)
- Easily switch between workflow managers (ROCOTO, ecFlow, etc.)
- Be extendable and flexible to keep up with evolving modeling system(s)
- Handle R2O transition for multiple modeling systems

Global Workflow keeps growing!





FV3GFS v15 (current ops)

FV3GFS v16 (pre-implementation)

Workflow configuration system

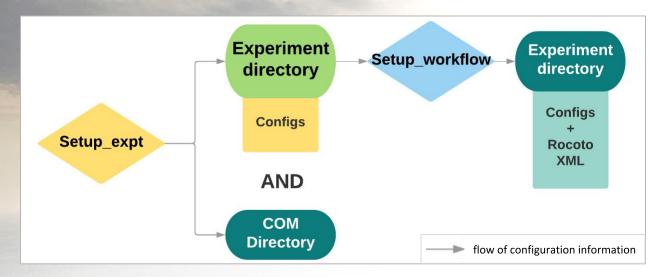
The major purpose of workflow configuration system is to enable the users to:

- Design and select the workflow structure.
- Pass through certain configurable variables into applications that are included in the workflow.

Successful workflow configuration systems include:

- User friendliness Easier for new users to set up a end-to-end workflow.
- Consistency Ensuring all components of workflow stay consistent with each other, eliminating a large portion of human errors.
- Accountability Easier documentation of completed experiment. Records would be archived in a more organized way.
- Extendability Easy to handle evolving modeling system enhancements.

Current Global Workflow Configuration System



Steps:

- Run setup_expt python script with numerous (and growing) command-line options
- Manually edit config files to settings for each program involved. These files are essentially pieces of shell scripts that will be "sourced" by the execution scripts at runtime.
- Run setup_workflow python script to generate ROCOTO XML

User friendliness?	Could be friendlier
Consistent?	Yes but limited to one model
Accountable?	Barely
Extendable?	Yes but not easy

What is CROW?

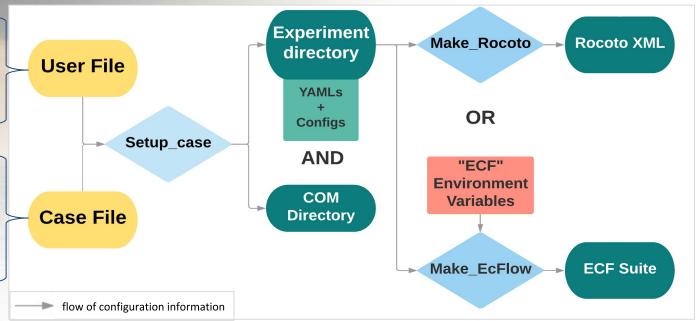
The "Configuration manager for Research and Operational Workflows" (CROW) is a python-based workflow toolbox that automates and streamlines the generation and configuration of NCEP workflows and connects system jobs to a workflow manager.

https://github.com/NOAA-EMC/CROW

CROW Configuration System global-workflow implementation

User file* = where a user defines their machine specific project codes and disk space to use (more info in later slide)

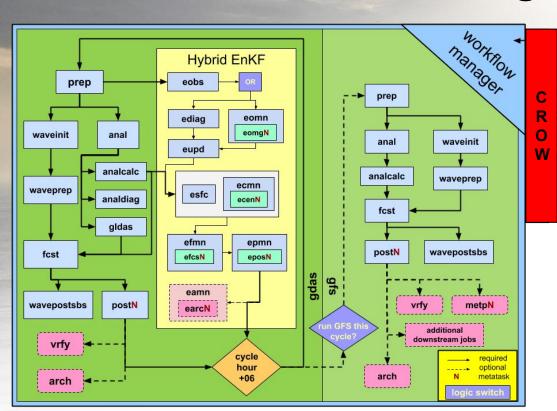
Case file* = the high-level configuration switches for an experiment; stock ones available for specific modes (more info in later slide)



^{*}user and case files can/will be implemented differently between apps

Round-cornered boxes are ASCII files at various stages; yellow color indicates places for user input, while dark green boxes are the final products. Diamonds are scripts run by the user.

How CROW fits with global-workflow



Repository structure:

(top)global-workflow

- docs : related documentations
- **fix**: Directory for fix files
- jobs: Top level job scripts (J_* job)
- modulefiles: modules to be loaded
- parm: templates for config
- **scripts**: driving scripts
- **sorc**: application source code
- **ush**: lower level scripts
- **util**: various utilities
- workflow: configuration system
 - CROW repository with setup and make scripts
 - background files
 - user file
 - case files

Benefits of CROW

Many benefits are behind the scenes at first:

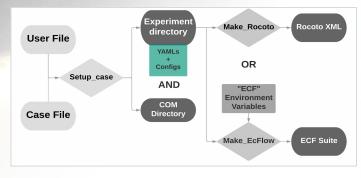
- Self-contained
- Smart
- Modularized
- Generalized

- Python based
- "Yamlized"

- -- unit test and regression test enabled
- -- validation of configuration settings
- -- easier troubleshooting (never easy, but easier)
- -- easier adding/removing jobs
- -- easier collaboration
- -- smoother R2O transition (now supports ecFlow)
- -- turn-key conversion of workflow manager
- -- cross-platform portable, even on a laptop
- -- shorter learning curve for new users

More to come in the future...

Background Files



To enable CROW-style configuration and provide an interface for CROW, a series of "background files" needs to be provided for a target modeling system (e.g. global-workflow). They can be located under a top-level directory named "workflow" within the target repository.

/schema task template, information of configurable variables (name, type, values)

/defaults default values for each group of variables

/layout workflow layouts associated with a certain modeling system

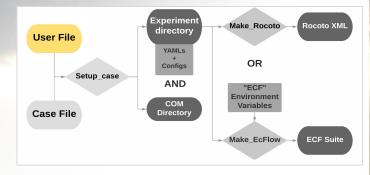
/config templates of all config files (a mirror of parm/config files in global-workflow)

/runtime one-step implemented task templates comparing to /schema/task.yaml

/platforms platform-related information. One file for each supported platform.

These files are ASCII text files formatted in YAML. They collectively serve as the interface between the modeling system and the CROW toolbox.

User File



The user file is where a user enters their user-specific information:

- user_places: user-specific locations and paths
 - EXPROOT: Designated place for experiment directory (EXPDIR)
- accounting: information needed to submit supercomputer job cards
 - cpu_project: cpu allocation group
 - hpss_project: hpss project code

user_places: &user_places

EXPROOT: /mnt/lfs3/projects/hfv3gfs/

accounting: &accounting

cpu_project: hfv3gfs

hpss_project: emc-global

Complete list of configurable variables can be found in the CROW documentation in GitHub.io page:

https://noaa-emc.github.io/CROW

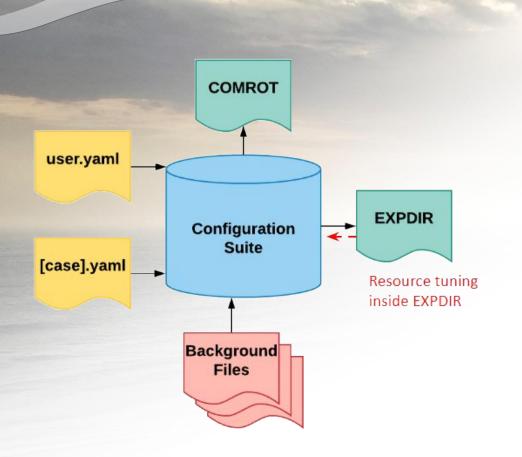
Case File

- fv3_settings: resolution and # of levels of deterministic forecast
- places: workflow configuration yaml file to use
- settings:
 - SDATE start date of experiment(YYYY-MM-DDtCC:mm:ss)
 - EDATE end date of experiment (YYYY-MM-DDtCC:mm:ss)
 - run_gsi whether to run data assimilation
 ('Yes' if cycling, 'No" if free-forecast mode)
 - chgres_and_convert_ics use when doing free-forecasts to run extra IC-making jobs
 - gfs_cyc frequency to run gfs long forecast

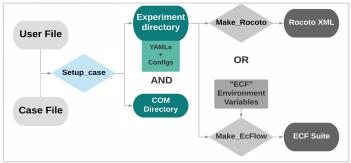
```
case:
    fv3_settings:
        CASE: C192
        LEVS: 65
    places:
        workflow_file: workflow/free_forecast_gfs.yaml
    settings:
        SDATE: 2019-05-01t00:00:00
        EDATE: 2019-05-01t06:00:00
        run_gsi: No
        chgres_and_convert_ics: Yes
        gfs_cyc: 4
```

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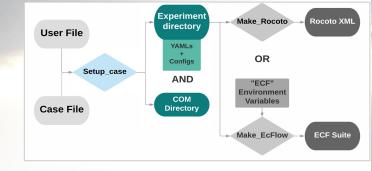


CROW YAML Step 1: Configuration



These steps happen under the hood in the CROW-HAFS implementation. These slides show an approximate implementation.

Step 1: Configuration



Step 1 establishes an experiment directory (EXPDIR) and a rotating output directory (COM a.k.a. ROTDIR) which contain the following:

- 1. EXPDIR: configuration files for each job in the workflow; these config files are built by parsing the system database based on the case file and populating templated configs with that information. The resulting configs are set for the request experiment design.
- 2. COM (a.k.a. ROTDIR): this is your rotating directory for model inputs and outputs, this naming convention comes from operations

Depending on your implementation of CROW this step may utilize a setup script called "setup_case.sh". More on this in the next slide.

Step 1: Configuration

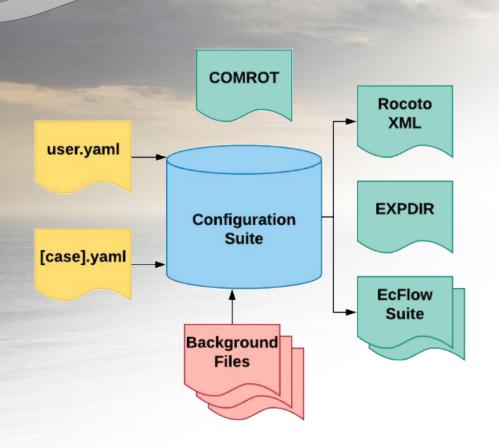
USAGE: setup_case.sh [options] \$CASE_NAME \$EXPERIMENT_NAME

CASE_NAME: a case name from the cases/ directory; can include ".yaml" part

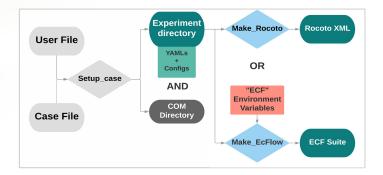
EXPERIMENT_NAME: your name for this execution. This string is used to decide where to put temporary and result files from the simulation. This must be alphanumeric and begin with a letter.

Additional options/flags:

-р \$НРС	specify platform name SHPC, required if multiple platforms available
-c	skip COM directory creation (recommend to use when making your own initial conditions)
-f/-F	force COM directory re-creation and overwrite experimental directory files (-F overwrites platform.yaml)
-V	verbose mode
-d / -D	debug mode / super debug mode
-m	using manual mode
	-v -d -D, more and more screen output during workflow generationD will slow down the process quite
	significantly. Only recommended for developers.
-S	sandbox mode.
	Enables workflow generation without supercomputer access. This option is developed for pure debugging purpose
	for CROW and workflow developers. When activated, CROW will skip platform validation. Ptmp, stmp and expdir will all be defined under PROJECT_DIR. User need to make sure writing access is granted for PROJECT_DIR.

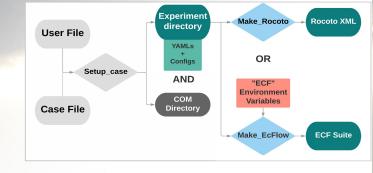


CROW YAML Step 2: Generation



These steps happen under the hood in the CROW-HAFS implementation. These slides show an approximate implementation.

Step 2: Generation



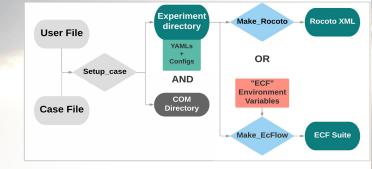
Step 2 generates the workflow manager files for your experiment. The files produced in step 1 are parsed to create the needed input files for the workflow manager you are utilizing.

Depending on your implementation there will be separate scripts for each workflow manager type. More on those in the next slide.

- ROCOTO an xml file for interacting with the scheduler and a sample crontab file for setting up unattended forward progress with cron
- ecFlow suite definition files for interacting with an ecFlow server which interacts with the scheduler

Additional workflow managers can be supported by CROW in the future.

Step 2: Generation



This will write a Rocoto xml file and a crontab file for recurring job. The usage and outcome is almost identical with the "setup_workflow.py" script of the legacy configuration system. However, instead of reading the config files, this file gets the configuration information totally by reading YAML configuration files under \$EXPERIMENT_DIRECTORY. So, modifying the config files in the experiment directory won't affect the outcome. Experiment directory config files are used by workflow jobs at run-time.

> make_ecflow_files_for.sh \$EXPERIMENT_DIRECTORY

Note: When running with ecFlow, the four "ECF" environment variables (\$ECF_HOME, \$ECF_ROOT, \$ECF_PORT and \$ECF_HOST) need to be properly set in your environment. (More details see ecFlow Training)

CROW YAML Reader

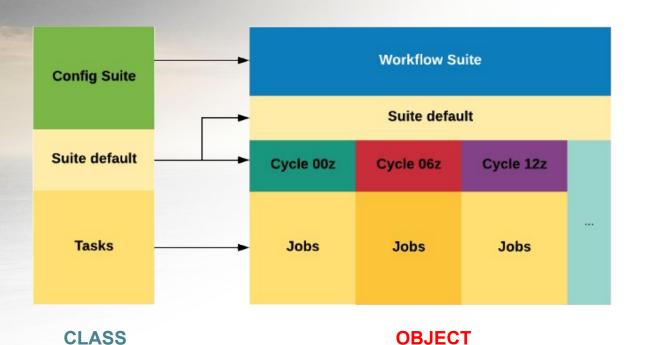
CROW Config CROW YAML Config Parser

Python data structure

```
my_crow_yaml:
    five: 5
    six: 6
    thirty: !calc five*six
    sixty: !calc thirt
    true: !calc thirt
    tomorrow: !timede
    htxt: hello
    wtxt: world
    hello_world: !expand "{htxt}
{wtxt}"
```

```
my crow yaml=eval dict({
 "five": 5,
 "six": 6,
 "thirty": strcalc("five*six"),
  "sixty": strcalc("thirty*2"),
  "true": strcalc("thirty<sixty"),
 "tomorrow": TimedeltaMaker("+24:00:00"),
 "htxt": "hello",
  "wtxt": "world",
  "hello world": strexpand("{htxt} {wtxt}")
  })
```

Workflow "task" and "job"



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Development of CROW - How/Where

CROW is open for development. Users can open issues and create pull requests here:

- Publicly available on GitHub:
 - https://github.com/NOAA-EMC/CROW
- Documentation being built:

https://noaa-emc.github.io/CROW/

Code managers and points of contact:

Jian Kuang (jian.kuang@noa.gov)

Kate Friedman (<u>kate.friedman@noaa.gov</u>)

Development of CROW - What

New capabilities currently being developed:

Workflow-level Hierarchical Testing Framework (HTF): This feature, under development, will enable CROW to orchestrate "dry-runs" of the workflow that it configures, an enhancement of the test capability of CROW.

CROW Implementations

The following are ongoing implementations of CROW at various stages:

global-workflow/FV3GFS: Introducing alongside current configuration system.

Ocean-DA: Data assimilation for global ocean simulation.

MOM6-CICE Coupling: Significant upgrade of the workflow and configuration systems need for upcoming operational coupled forecast system.

HAFS: Next generation hurricane forecast system for NCEP.

Community Support

Beyond collaborative efforts through the GitHub repository this is still mostly TBD.

Need community input on this!

Thank you! Questions?