4

ESM-Tools Terminology

Overview
YAML Hierarchy
Configuration files
Runscripts
YAML Sections
Feature Variables
Compilation Scripts
.run files

4 Terminology

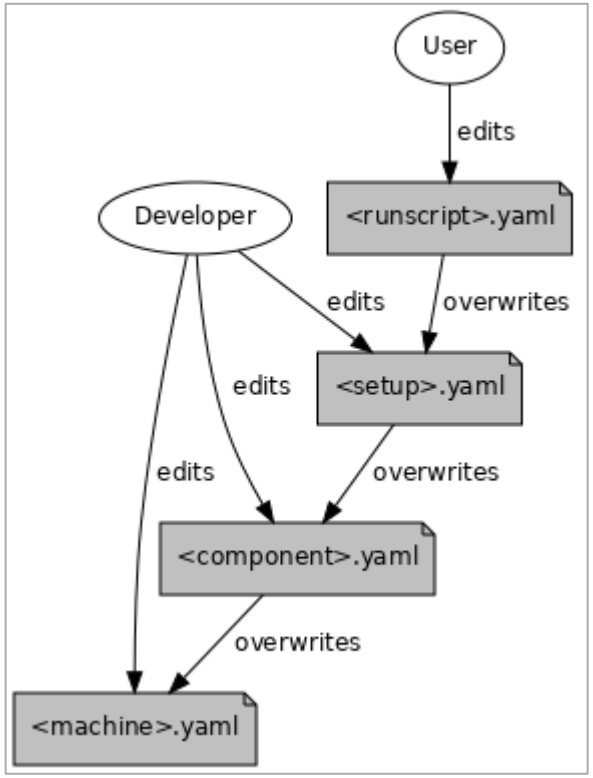
- Through out this workshop we will be using ESM-Tools-specific terms that you'll need to be familiar with. Those terms are defined in this power point.

- You'll see those terms in the other slides coloured in orange

4 YAML Hierarchy

YAML files are always inherited from more general to more specific. Last one wins (eg. user runscript).

File Name	Order of Execution	Precedence	Location	Defined by
machine.yaml	First	Lowest	esm_tools/configs/machines	ESM-Tools
model.yaml			esm_tools/configs/components	ESM-Tools
setup.yaml			esm_tools/configs/setup (Note: when using a coupled setup)	ESM-Tools
runscript.yaml	Last	Highest	user defined directory	User



4 Terminology – configuration files

The yaml files that contain the **default configurations** for HPCs, models, coupled systems, job schedulers (SLURM, PBS), default ESM-Tools recipes, …

```
esm_tools/configs/
├── components
├── setups
├── machines
├── coupling
├── default
├── esm_software
└── other_software
```

components	Stand-alone model, couplers, I/O libraries configurations
setups	Coupled system default configurations
machines	HPC default configurations
coupling	Source code branch information for coupled system stored here, only for use in ESM-Master (to be removed in the future)
default	ESM-Tools default configurations
esm_software	Recipes and defaults for ESM-Runscripts and ESM-Master
other_software	Job schedulers and other external software configurations

4 Terminology – runscripts

- User interface for running experiments
- Should include all the deviations from the defaults defined in the **configuration files**
- Can be shared to reproduce the same experiment
- A yaml file with **sections**

<your_fesom_runscript>.yaml

```yaml
general:
        account: <your_account>
        setup_name: fesom
        compute_time: "00:20:00"
        initial_date: '2001-01-01'
        final_date: '2001-03-01'
        base_dir: <your_basedir>
        nyear: 0
        nmonth: 1
        nday: 0
        use_venv: False
fesom:
        version: 2.1
        model_dir: <your_model_dir>
        lresume: 0
        restart_rate: 1
        restart_unit: 'm'
        post_processing: 0
```

4 Terminology – YAML sections

- 1st level keys on a yaml file
  - general
  - <model_name>/<component_name>
  - computer

- Only the **runscripts** and the **setups** files have **sections**

```
runscripts
configs
        components
        setups
        machines
        coupling

        default
        esm_software
        other_software
```

<your_fesom_runscript>.yaml

```yaml
general:
        account: <your_account>
        setup_name: fesom
        compute_time: "00:20:00"
        initial_date: '2001-01-01'
        final_date: '2001-03-01'
        base_dir: <your_basedir>
        nyear: 0
        nmonth: 1
        nday: 0
        use_venv: False
fesom:
        version: 2.1
        model_dir: <your_model_dir>
        lresume: 0
        restart_rate: 1
        restart_unit: 'm'
        post_processing: 0
```

4 Terminology – feature variables

Some variables in the yaml files trigger functionalities in ESM-Tools. Through this variables the **yaml syntax is extended**.

We refer to this variables as **feature variables**

```yaml
# time variables
general:
    nday: 0
    nmonth: 1
    initial_date: "1850-01-01T00:00:00"
    final_date: "1860-01-01T00:00:00"
```

```yaml
# creating and accessing variables from different sections
ini_restart_dir: "${general.ini_restart_dir}/fesom/"
```

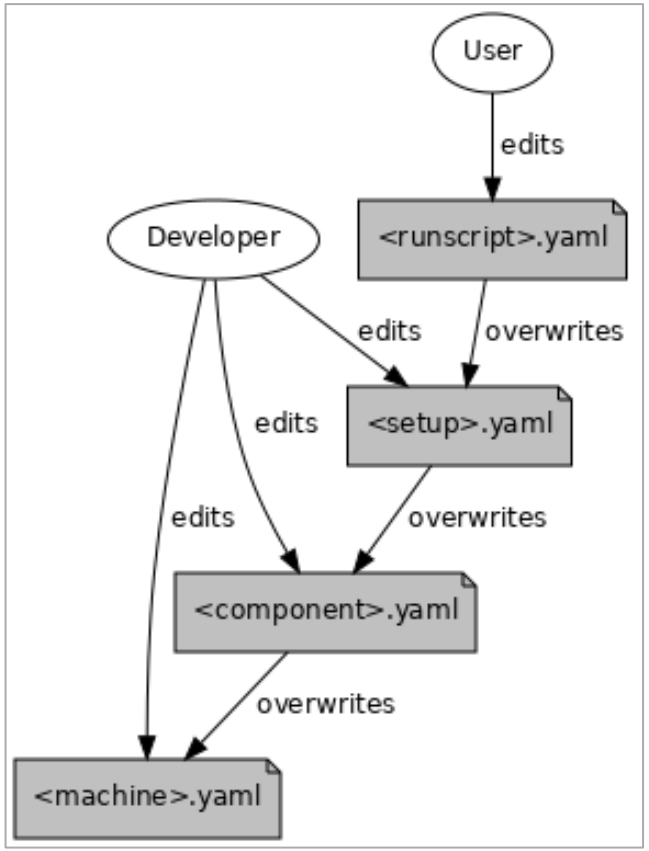
```yaml
# Changing Fortran namelists
namelist_changes:
    namelist.echam:
        runctl:
            out_expname: ${general.expid}
            dt_start:
                - ${pseudo_start_date!year}
                - ${pseudo_start_date!month}
```

```yaml
# adding and removing elements from lists and dicts

list1:
    - element1
    - element2

add_list1:
    - element3
    - element4
```

```yaml
# choose_ blocks allow select-case (aka switch) statements
resolution: CORE2

choose_resolution:
    CORE2:
        nx: 126858
        mesh_dir: "${pool_dir}/meshes/mesh_CORE2_final/"
        nproc: 288
        time_step: 450
    GLOB:
        nx: 830305
```

4 Terminology – finished_config file

- Internally, esm_parser puts together all the information from the different yaml files for the given experiment into a Python object called config
- This object, containing all the information about the experiment, is passed to the different ESM-Tools functions
- esm_runscripts dumps this object into a yaml file in `<experiment_dir>/run_DATE/configs/*finished_config.yaml` for runs that have not being submitted or are still running, or in `<experiment_dir>/configs/*finished_config.yaml` for runs that have already run
- The **finished_config file** is used for checking that the final configuration works as expected



4 Terminology – compilation scripts

- For each component that **esm_master** builds, it produces a compilation script **comp-*.sh** that includes the environment specified in the configuration files (machine + components + setups) files involved
- Written in the same directory where you execute **esm_master**
- Copied to the compilation folder after the building finishes

```
#!/bin/bash -l
# Dummy script generated by esm-tools, to be removed later:
set -e
module purge
module unload netcdf_c
module unload intel intelmpi
module load python3/2021.01-gcc-9.1.0
module load cmake/3.13.3
module load autoconf/2.69
module load nco
module load cdo
module load gcc/4.8.2
module unload intel intelmpi
module load intel/18.0.4 intelmpi/2018.5.288
module load libtool/2.4.6
module load automake/1.14.1
module unload gcc
module load gcc/4.8.2
export LC_ALL=en_US.UTF-8
export FC=mpiifort
export F77=mpiifort
export MPIFC=mpiifort
export CC=mpiicc
export CXX=mpiicpc
export MPIROOT="$(mpiifort -show | perl -lne 'm{ -I(.*?)/include } and print $1')"
...
cd fesom-2.1
mkdir -p build; cd build; cmake -DFESOM_COUPLED=ON ..; make install -j `nproc --all`
cd ..
```

4 Terminology –*.run files

- esm_runscripts produces a ***.run** script with SBATCH headers that is then submitted to SBATCH. This script contains the combined environments specified in the configuration files (machine + components + setups) files involved

- This script can be found in <experiment_dir>/run_DATE/scripts for runs that have not being submitted or are still running, or in the <experiment_dir/scripts> directory for runs that have already run

```
#SBATCH --partition=compute
#SBATCH --time=01:45:00
#SBATCH --ntasks=896
...
module purge
module unload netcdf_c
module unload intel intelmpi
...
export LC_ALL=en_US.UTF-8
export FC=mpif90
export F77=mpif90
...

# Set stack size to unlimited
ulimit -s unlimited

# 3...2...1...Liftoff!
echo $(date +"%a %b  %e %T %Y") : compute 1 1850-01-01T00:00:00 1233 - start
>> /work/ab0995/a270152//workshop_test/log//workshop_test_awiesm.log

cd /work/ab0995/a270152//workshop_test/run_18500101-18501231/work/

time srun -l --kill-on-bad-exit=1 --cpu_bind=cores --multi-prog hostfile_srun
2>&1 &

...
```

Terminology – check mode

- **esm_master** and **esm_runscripts** can run in check mode by adding the --check or -c flags to the command

- esm_master in check mode
  - Outputs the git commands and building commands but does not produce the **comp-*.sh** files

To be changed in the future to it procudes **comp-*.sh** files

- **esm_runscripts** in check mode
  - Bakes the yaml information and produces the **finished_config.yaml**
  - Prepares the experiment folder (copies in input, forcing, binaries, …)
  - Produces the ***.run** file
  - **Does not** submit the ***.run** script to sbatch

Terminology – models and components

FESOM-2

- AWI's ocean model
- Finite Volume
- Unestructure mesh

AWI-ESM-2.1

- ECHAM6 + FESOM-2.1 with OASIS3MCT
- Dynamic vegetation
- + REcoM (biogeochemistry) + PISM (WIP, offline coupled)

VILMA-PISM

- Offline coupling through ESM-Tools workflow manager