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EXCELENCIA SEVERO OCHOA

Reproducible science at large scale within a continous delivery pipeline: the BSC vision

Miguel Castrillo

BSC-ES Computational Earth Sciences

15/10/2019

ECMWF workshop: Building reproducible workflows for Earth Sciences

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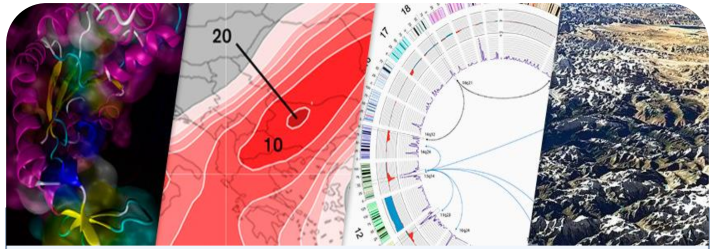
BSC-CNS objectives

Supercomputing services
to Spanish and EU researchers



R&D in Computer, Life, Earth and
Engineering Sciences

PhD programme, technology
transfer, public engagement

BSC-CNS is a consortium that includes

Spanish Government	60%	Gobierno de España · Ministerio de Ciencia, Innovación y Universidades
Catalan Government	30%	Generalitat de Catalunya Departament d'Empresa i Coneixement
Univ. Politècnica de Catalunya (UPC)	10%	Universitat Politècnica de Catalunya BarcelonaTech

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MareNostrum 4

Total peak performance: **13,7** Pflops

General Purpose Cluster:	11.15 Pflops	(1.07.2017)
CTE1-P9+Volta:	1.57 Pflops	(1.03.2018)
CTE2-AMD:	0.52 Pflops	(1.11.2019)
CTE3-Arm V8:	0.5 Pflops	(????)

PRACE

Access: prace-ri.eu/hpc_acces

RES
RED ESPAÑOLA DE SUPERCOMPUTACIÓN

Access: bsc.es/res-intranet

BSC
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MareNostrum 1
2004 – 42,3 Tflops
1st Europe / 4th World
New technologies

MareNostrum 2
2006 – 94,2 Tflops
1st Europe / 5th World
New technologies

MareNostrum 3
2012 – 1,1 Pflops
12th Europe / 36th World

MareNostrum 4
2017 – 11,1 Pflops
2nd Europe / 13th World
New technologies

MareNostrum 5. A European pre-exascale supercomputer

- **200 Petaflops** peak performance (200 x 10^{15})
- **Experimental platform** to create supercomputing technologies “made in Europe”
- **223 M€** of investiment

EuroHPC
Joint Undertaking

Hosting Consortium:

Spain Portugal Turkey Croatia

European Commission

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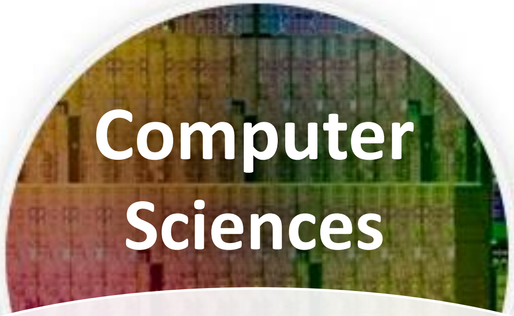
Generalitat de Catalunya
Departament d'Empresa i Coneixement

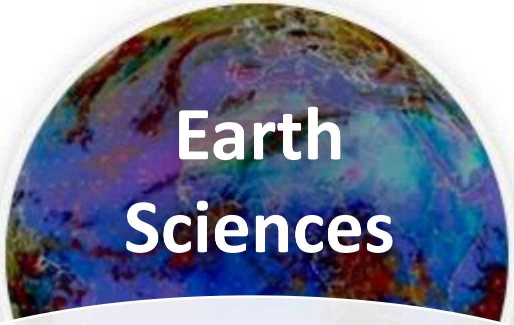
GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Mission of BSC Scientific Departments



To influence the way machines are built, programmed and used: programming models, performance tools, Big Data, computer architecture, energy efficiency



To develop and implement global and regional state-of-the-art models for short-term air quality forecast and long-term climate applications

To understand living organisms by means of theoretical and computational methods (molecular modeling, genomics, proteomics)

To develop scientific and engineering software to efficiently exploit super-computing capabilities (biomedical, geophysics, atmospheric, energy, social and economic simulations)

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Earth Sciences

Environmental modelling and forecasting, with a particular focus on weather, climate and air quality

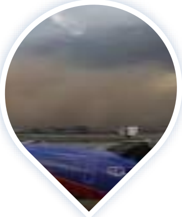
Research and Forecasts

Service Users Sectors


Infrastructures


Solar Energy


Urban development


Transport


Wind Energy


Agriculture


Insurance

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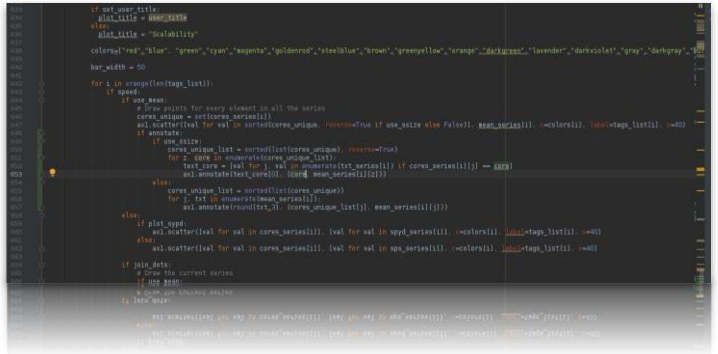
The Models & Workflows team

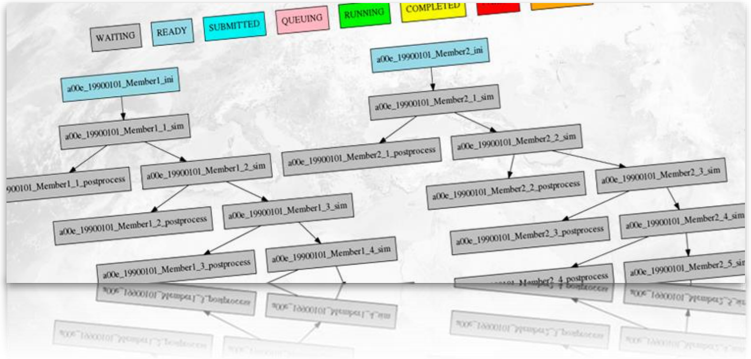
Models

Design, development, and deployment of Earth science **models** in close **collaboration** with the **scientific** groups aiming to understand and better predict the behaviour of Earth systems.

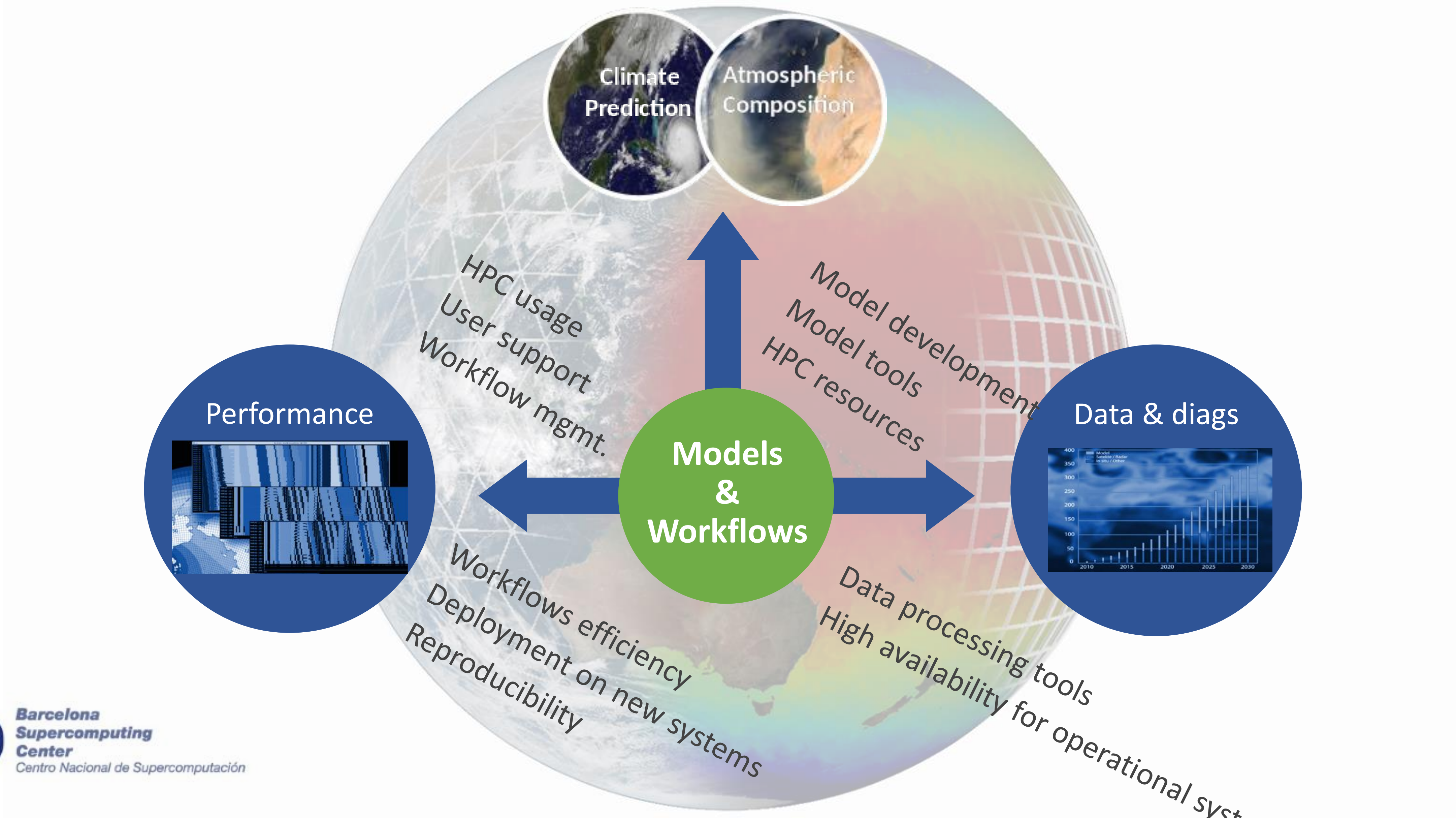
Workflows

Research and development of **methodologies** and **tools** that allow the **running** of scientific models in **production** and taking advantage of the increasing availability and variety of computing resources.





MWT synergies



High Performance Computing in Earth Sciences

- Earth System Models (ESMs) are sophisticated tools with continuously increasing complexity:
    - More components of Earth System are included
    - Finer Spatial and Temporal resolutions
- This increase in complexity could be developed thanks to the important parallel advances in HPC

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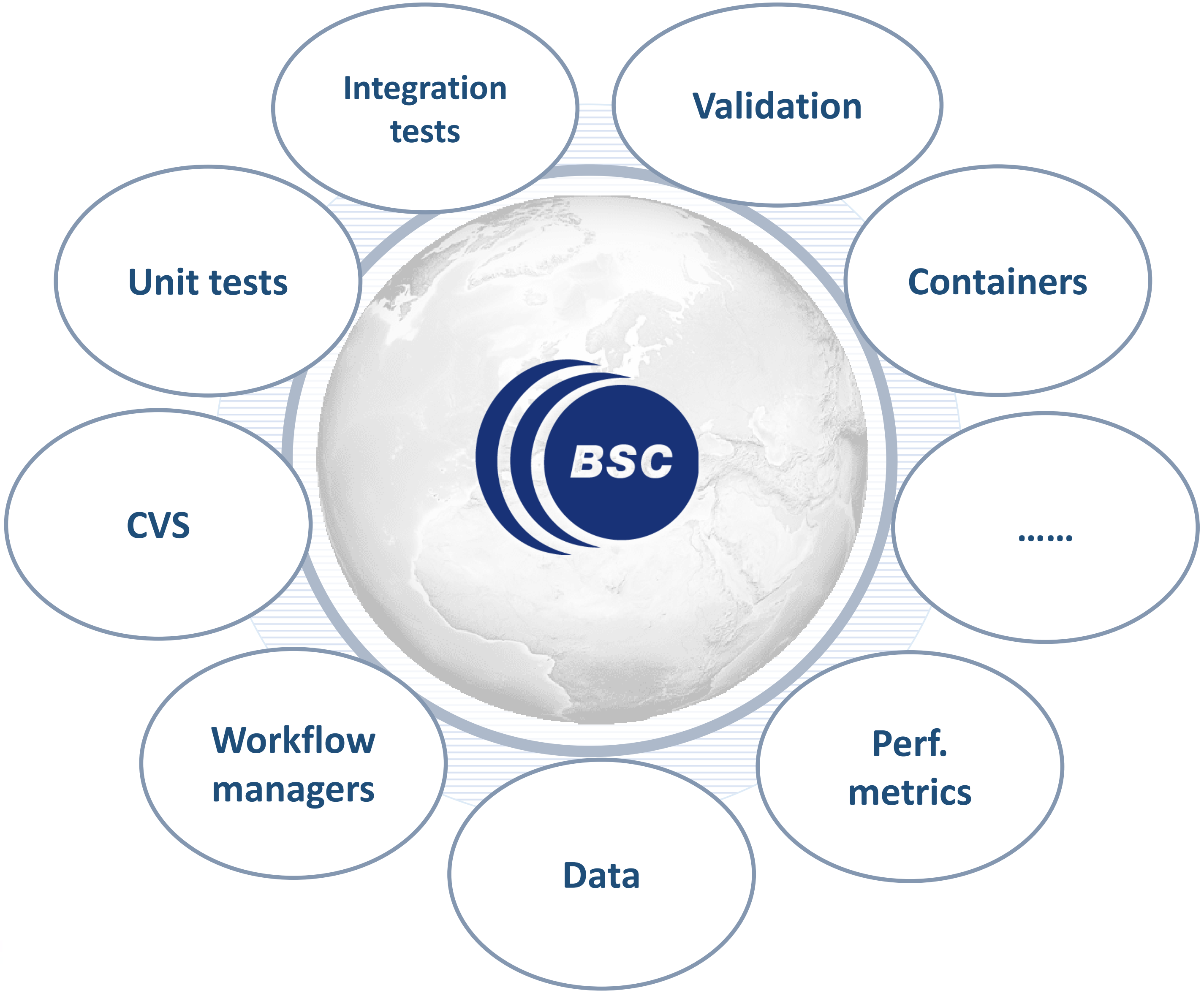
Workflows at BSC-ES



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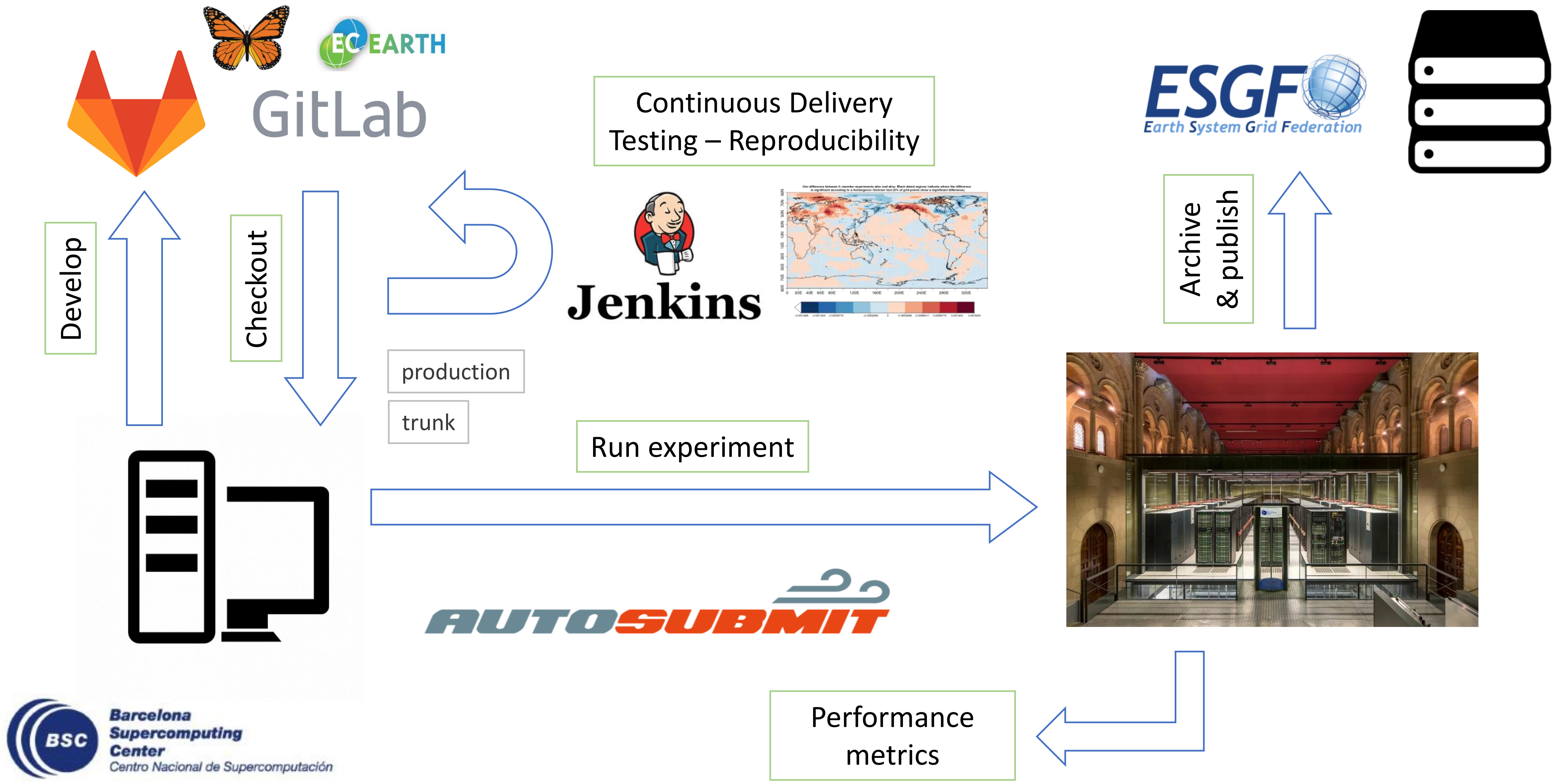
Our workflow



A workflow for ESM experiments

Model setup

- Configure experiment
- Set up platform-specific files
- Prepare run scripts

Deployment on remote HPC

- Tar and send model files / Synchronize updated files
- Compile the model

Initial data pre-processing

- Choose and deploy the initial data
- Pre-process initial conditions / restarts

Simulation

- Find a proper domain decomposition
- Run simulation
- Assimilation / synchronize jobs

Output data post-processing

- Post-process / normalize output data
- Archive restarts / output files
- Transfer results to local

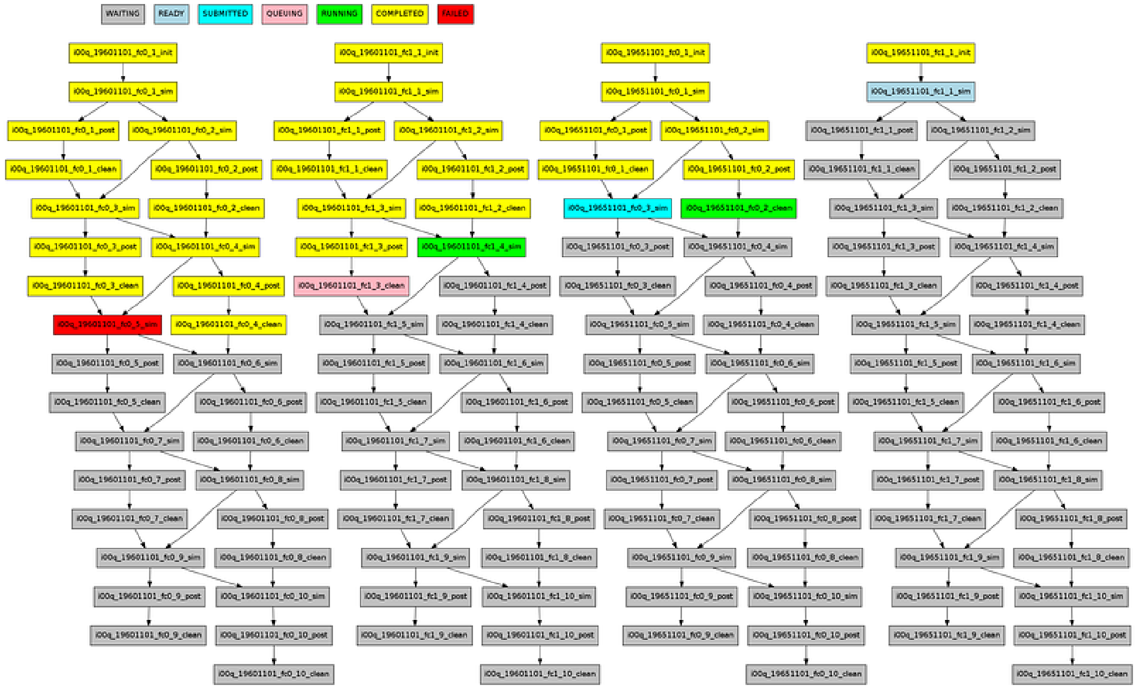
Verification & diagnostics

- Generate diagnostics
- Generate plots

Workflow managers: motivation

Workflow managers are **essential** to carry out production experiments in an **efficient** way

- Deal with workflow **complexity**
- Ensure **robustness** & **portability**
- **Usability** → Scientists more productive



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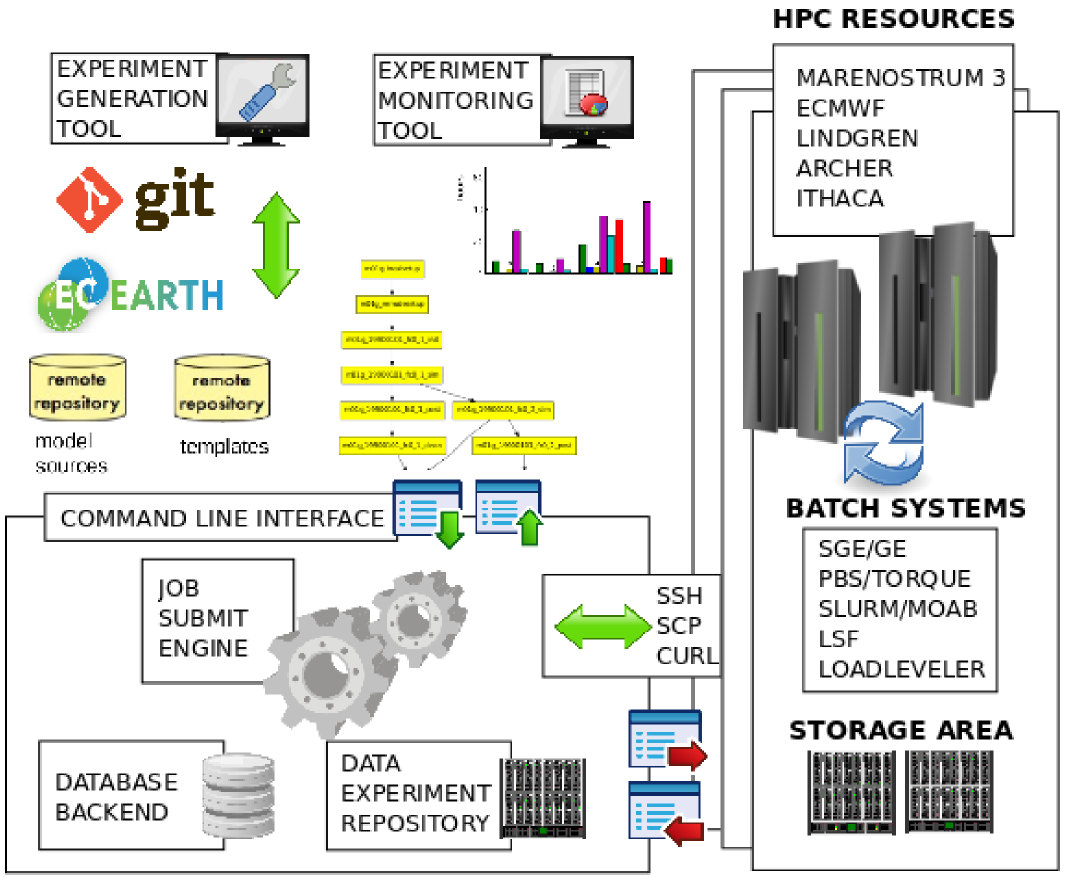
Autosubmit

A **versatile** tool to manage Weather and Climate Experiments in diverse Supercomputing Environments:

https://pypi.python.org/pypi/autosubmit



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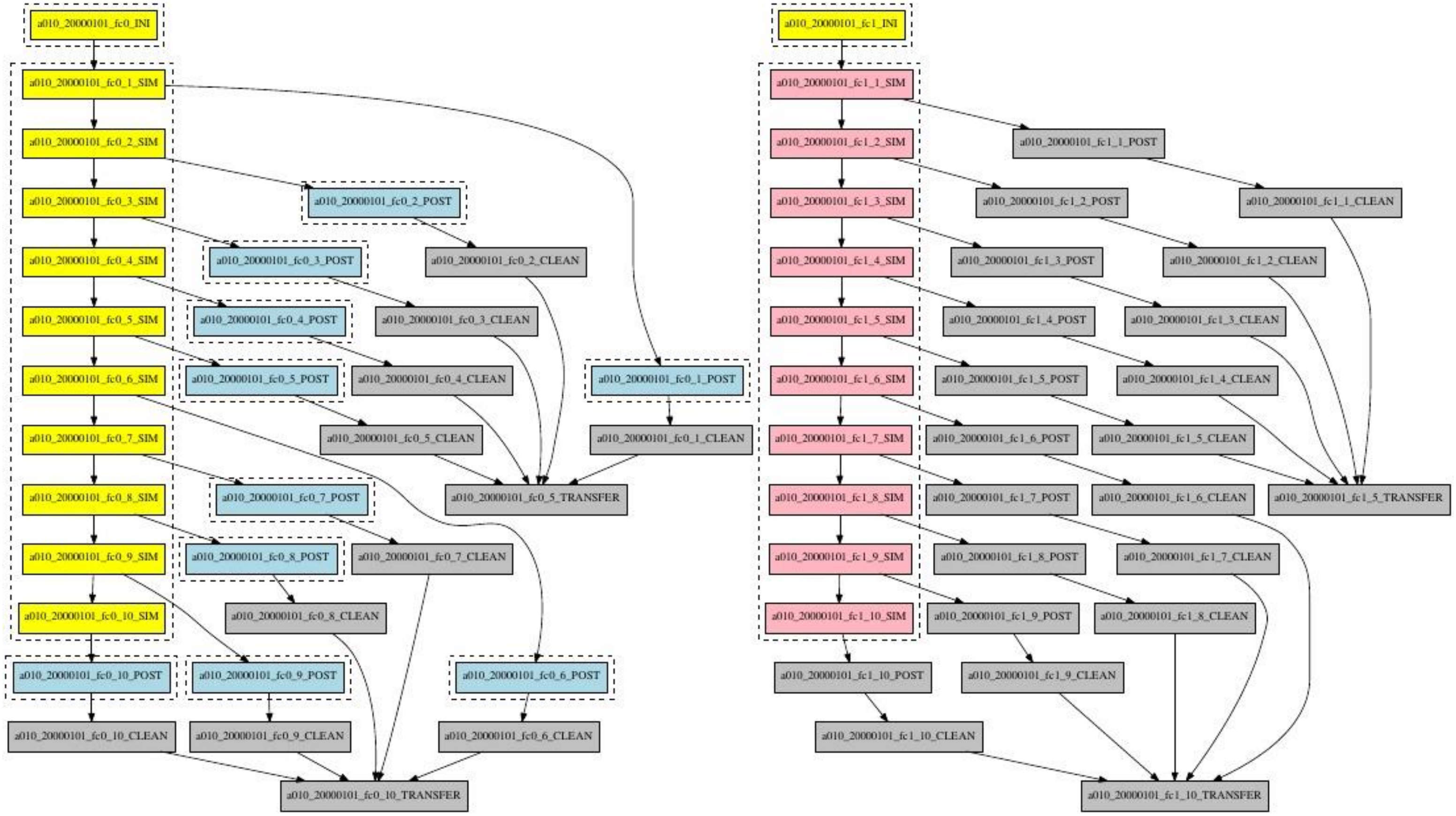
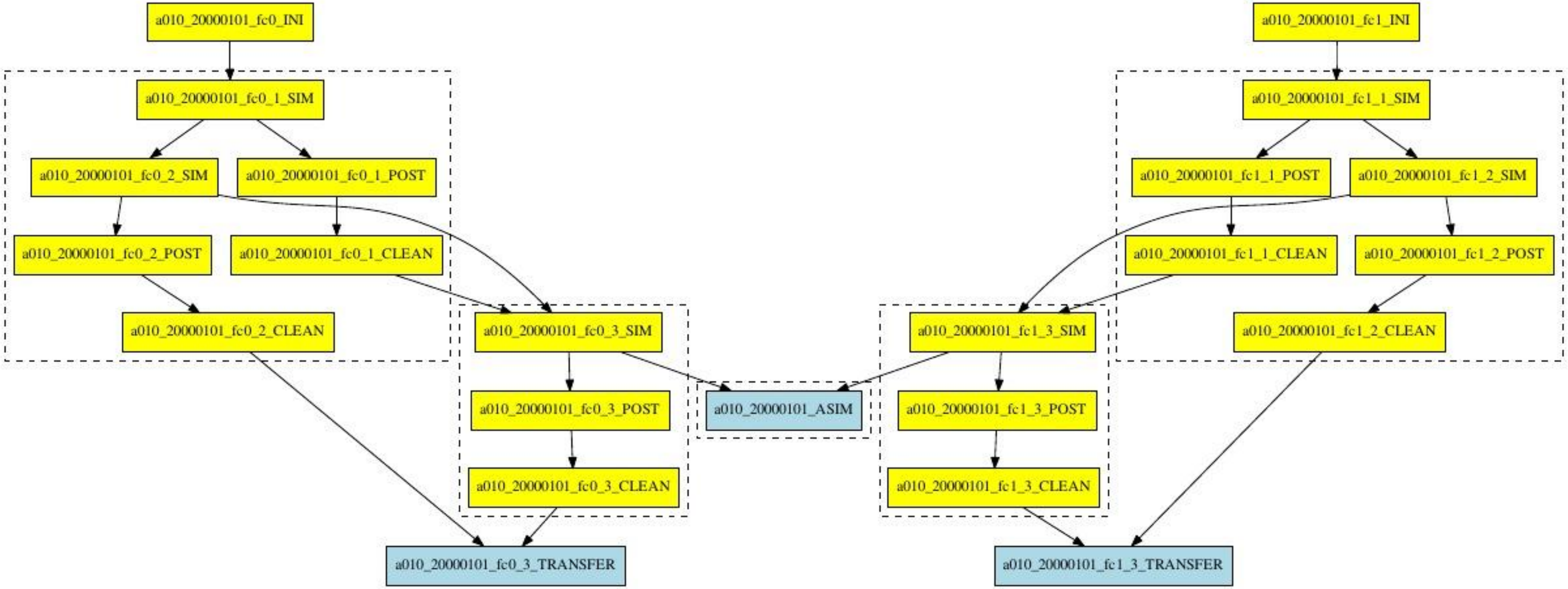
Autosubmit wrapper

Reducing queueing times by wrapping different jobs together



Autosubmit wrappers

Hybrid wrappers



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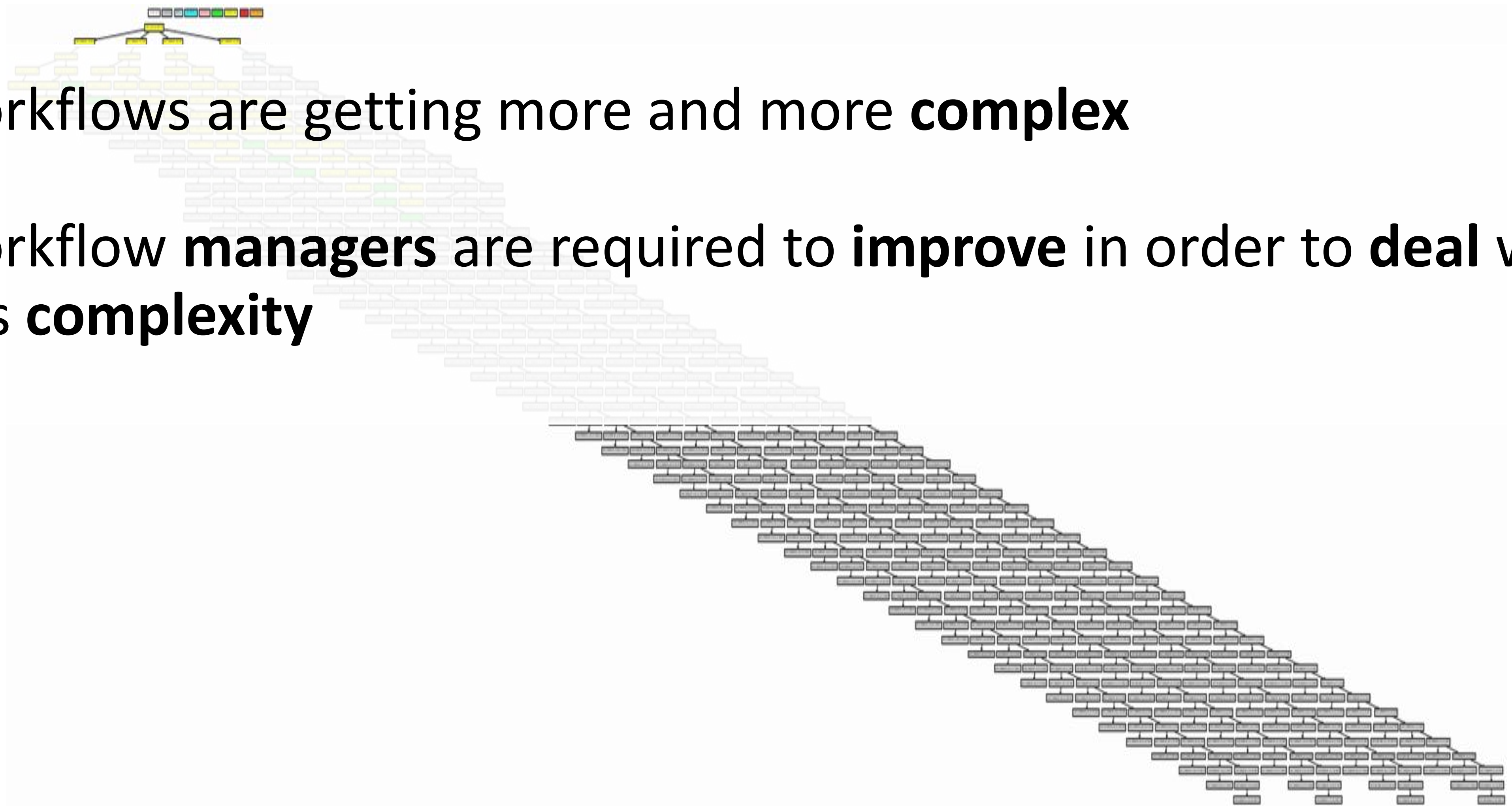
Autosubmit: lessons learned



- Workflows are getting more and more **complex**
- Workflow **managers** are required to **improve** in order to **deal** with this **complexity**

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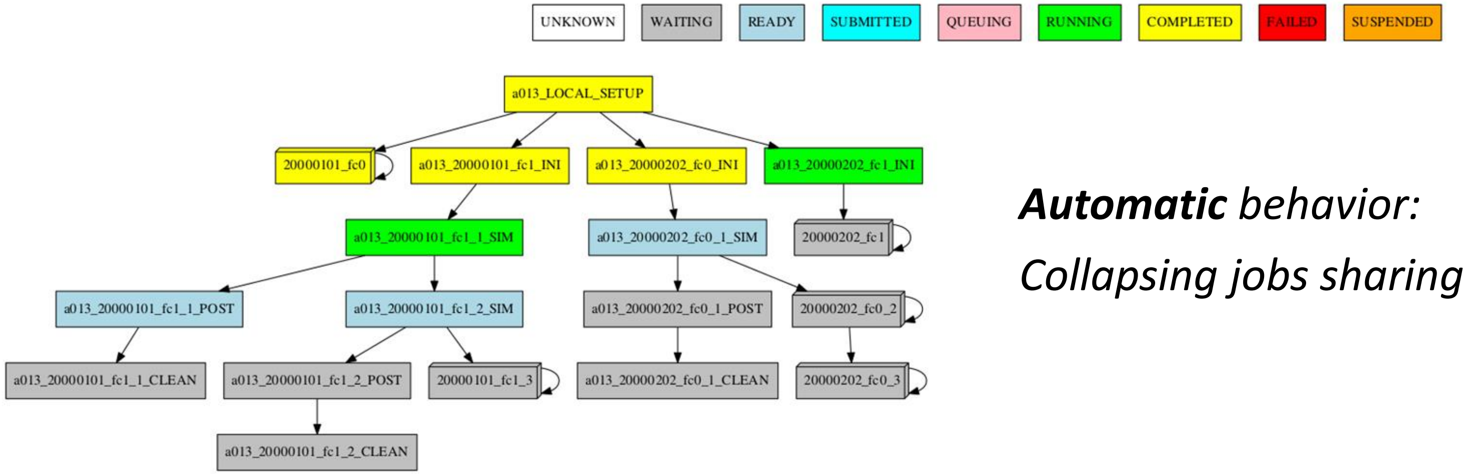
Autosubmit visualization

Grouping jobs by date, member, chunk, split; or automatically.

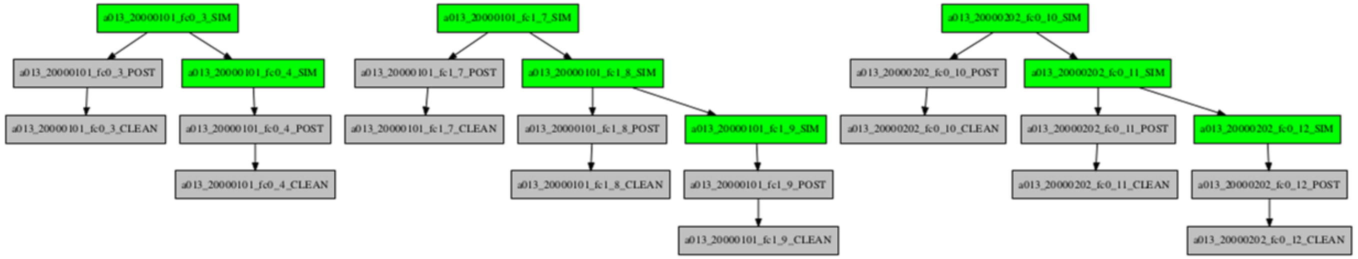


__Automatic__ behavior:

Collapsing jobs sharing status.

Hide groups:

Showing the more __relevant__ information.



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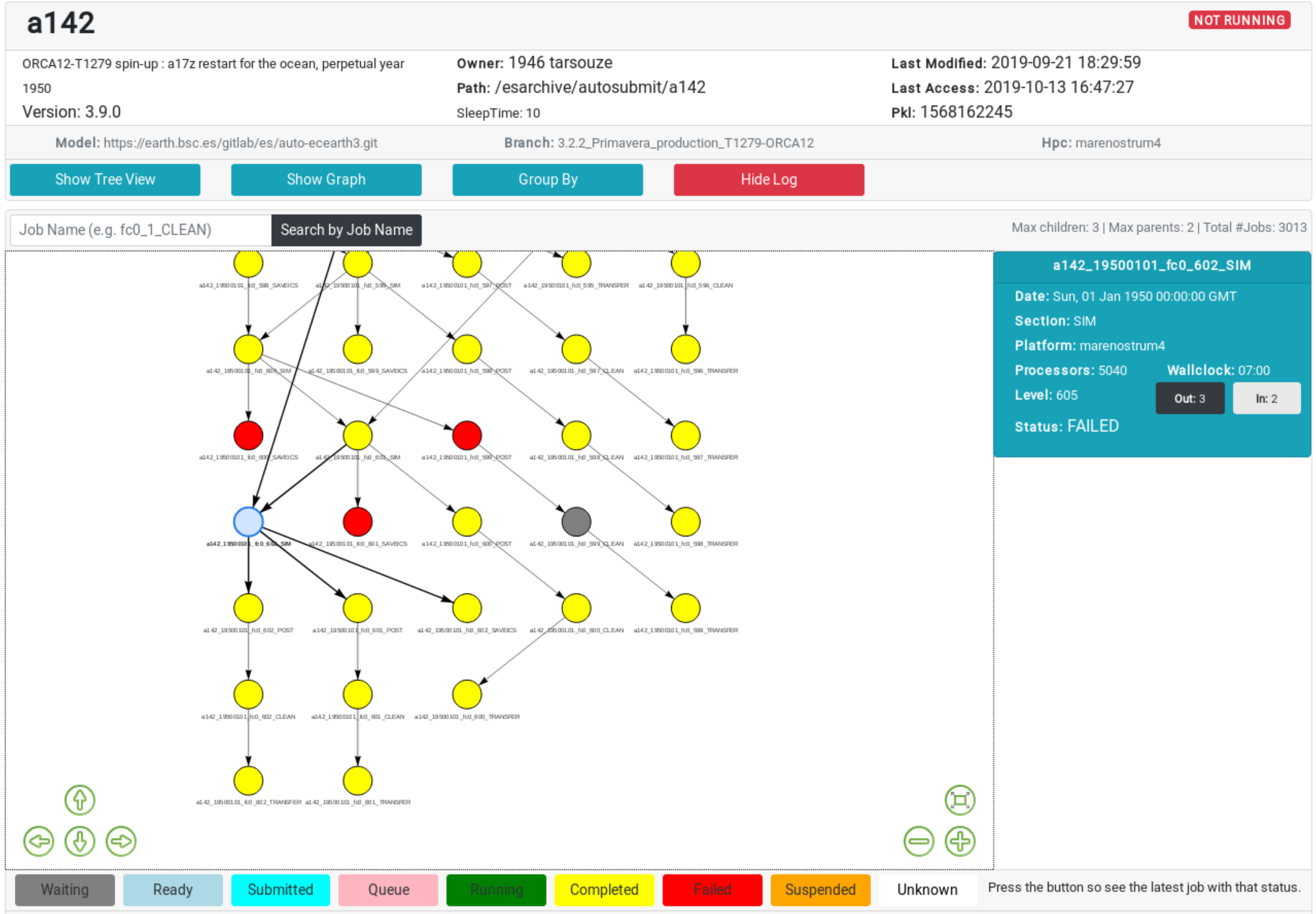
Autosubmit GUI



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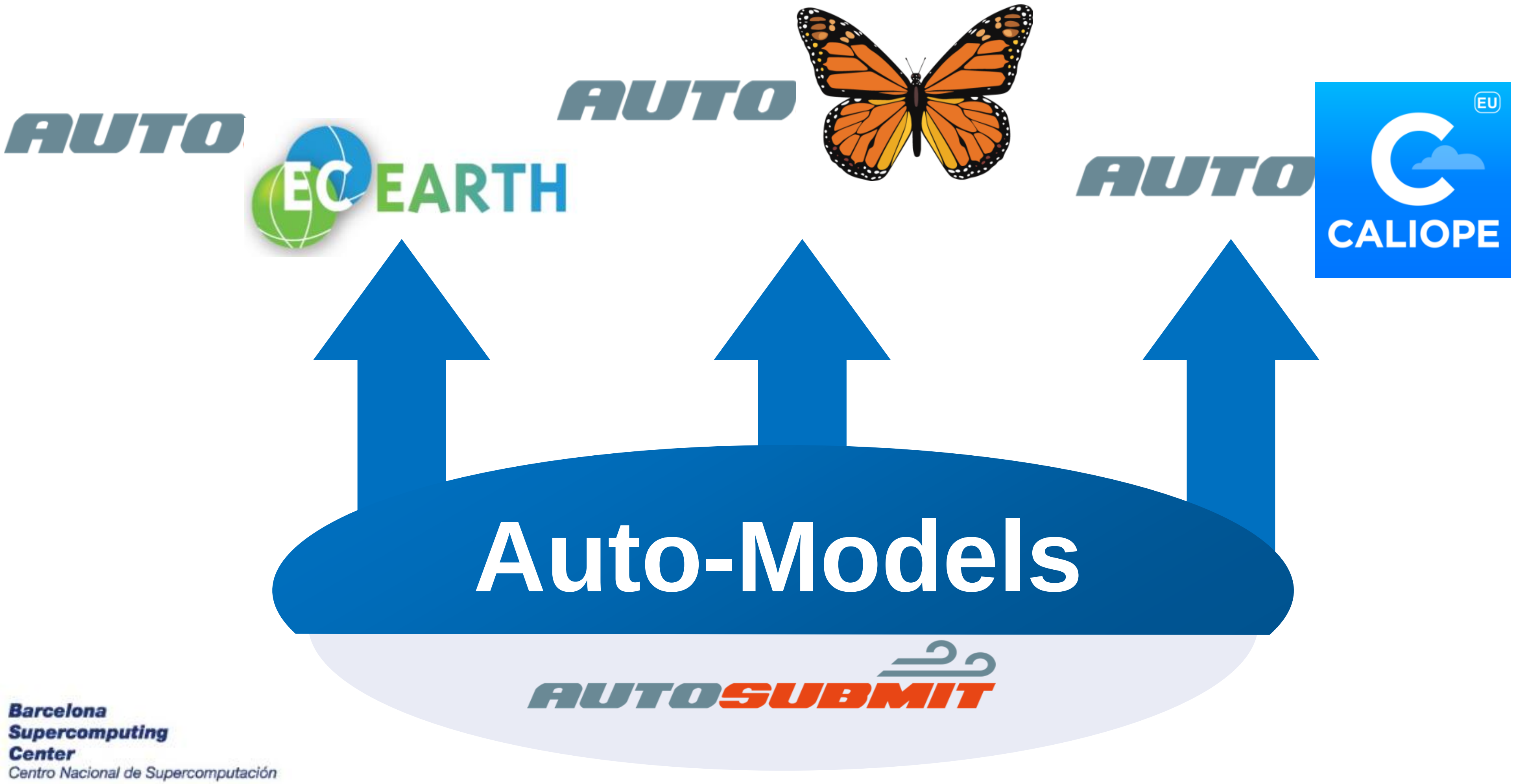
Auto-Models

Autosubmit + Model source + Job templates + Auxiliary functions + Utilities

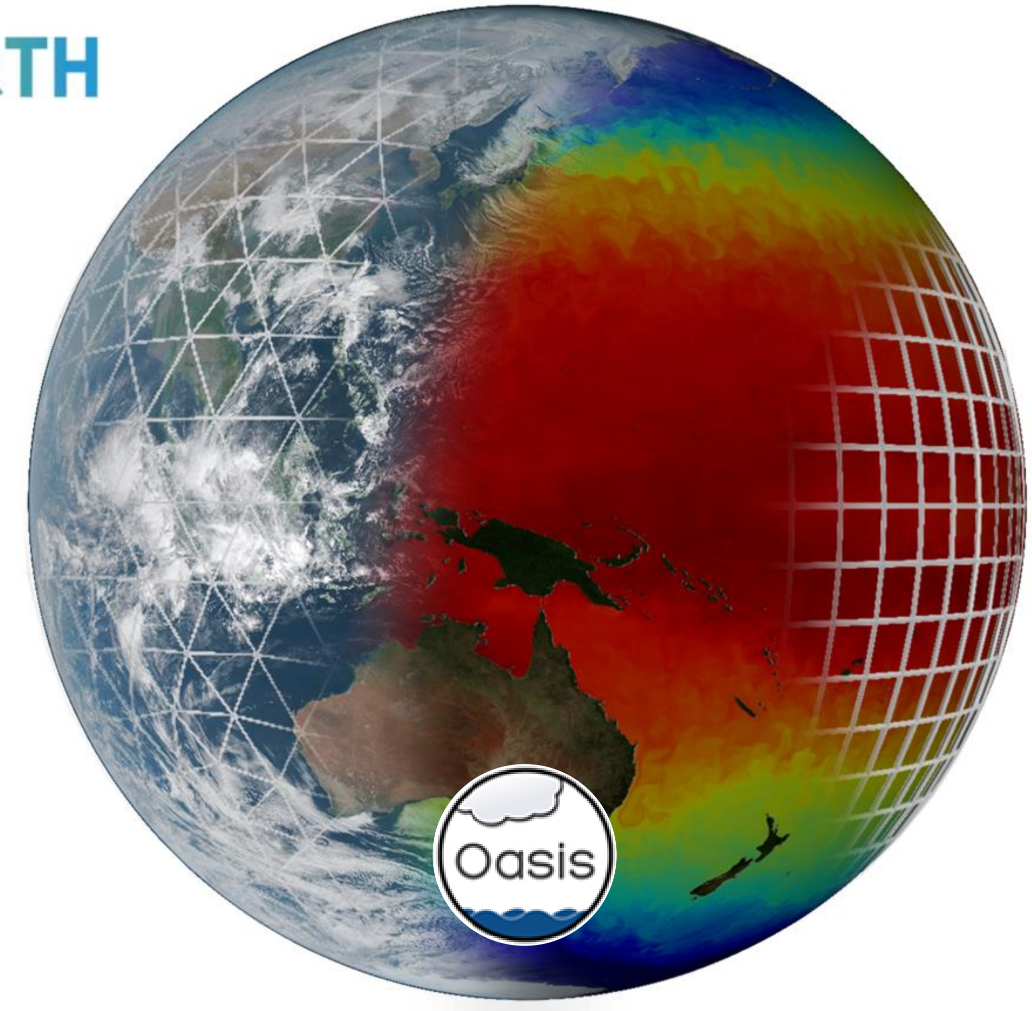


The EC-Earth ESM

Atmosphere:

IFS

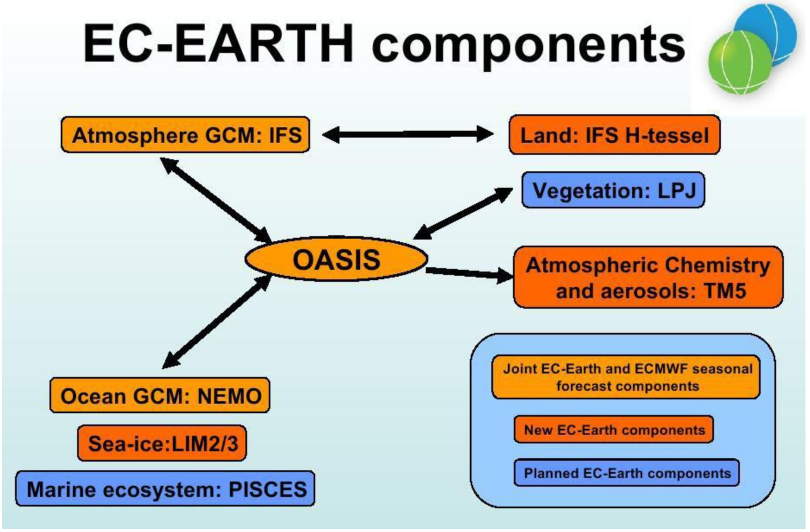
ECMWF



Ocean+ICE:

NEMO

Coupler:



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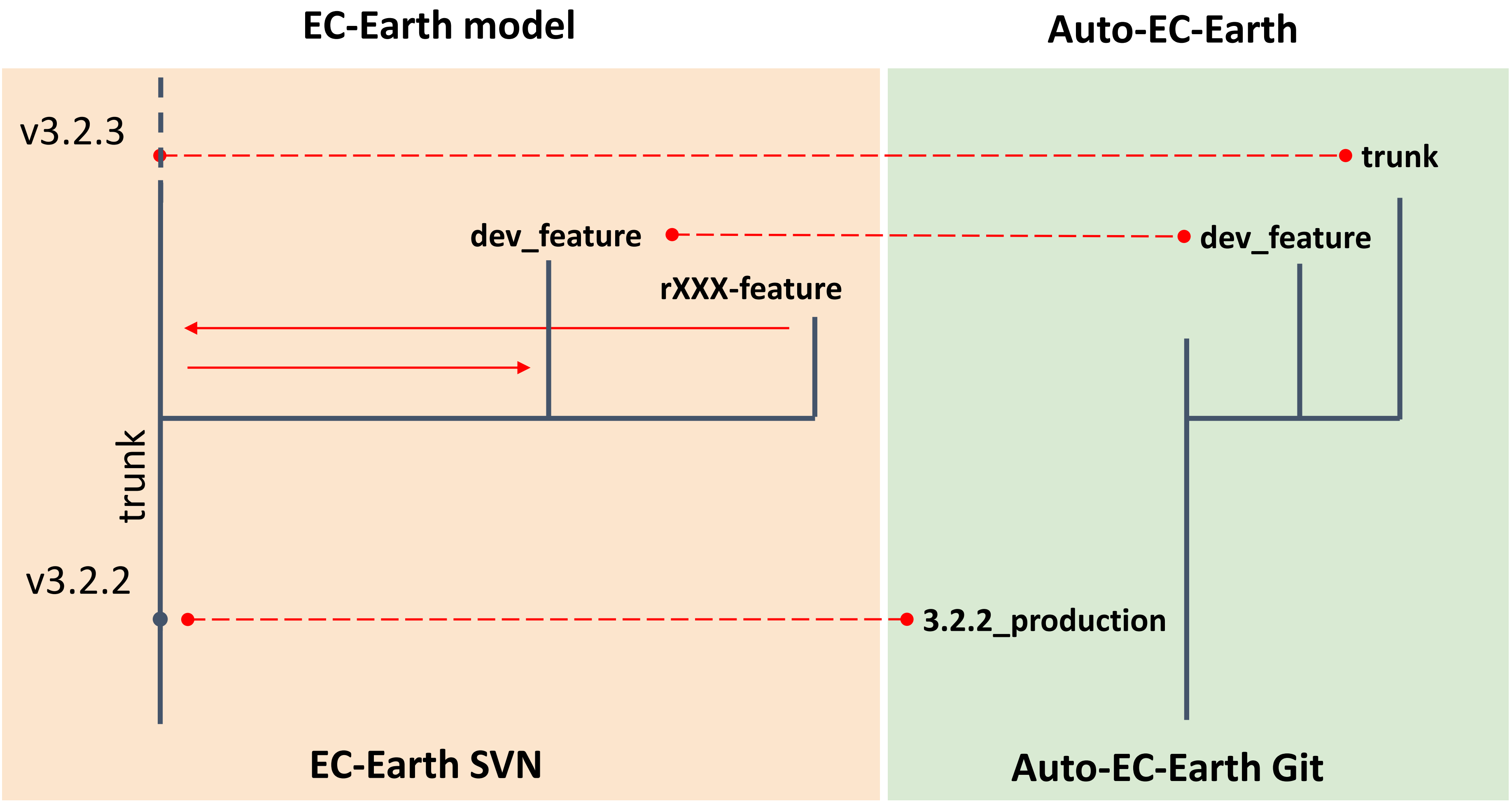
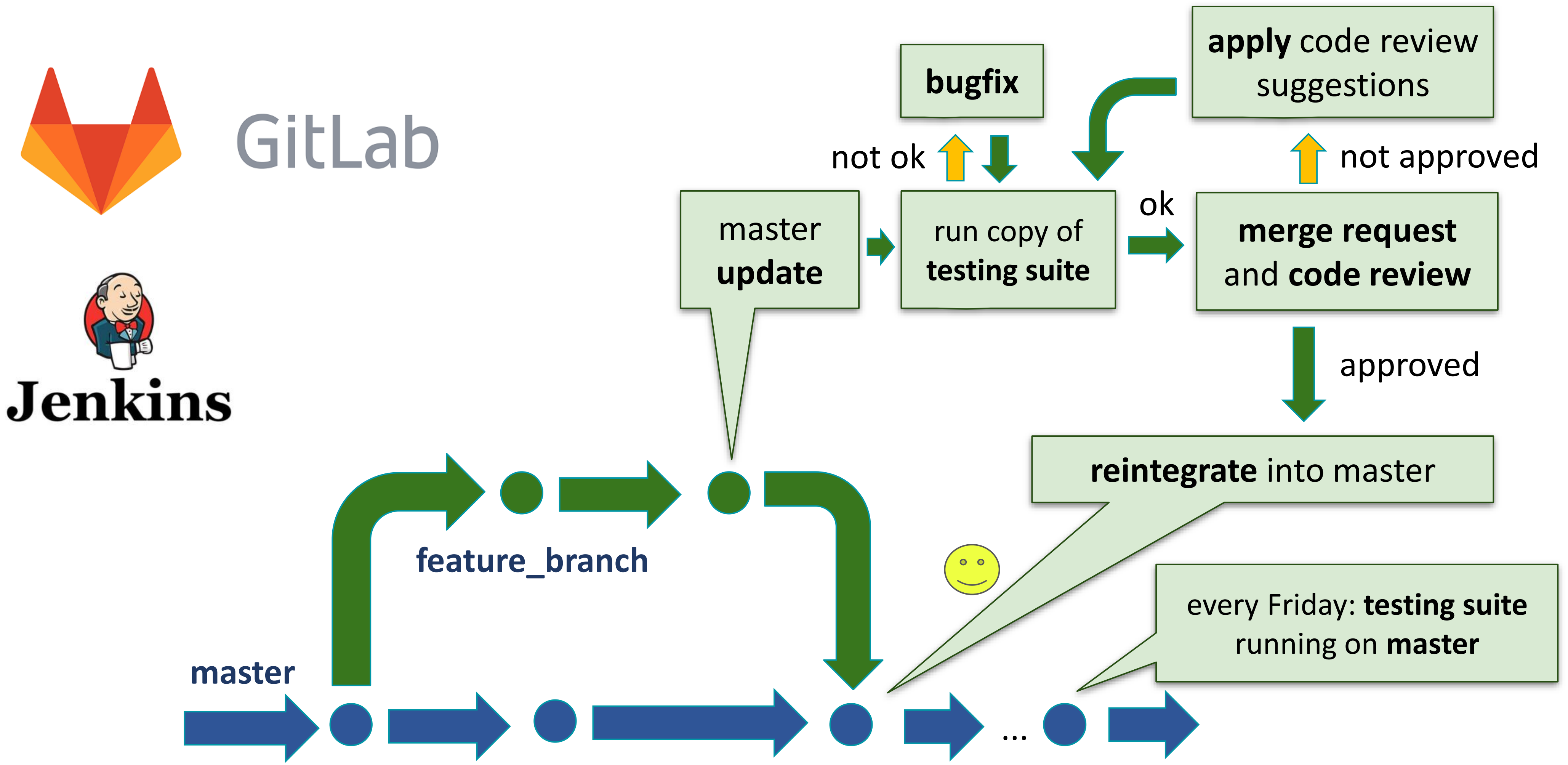
Auto-EC-Earth branching



Auto-Models development



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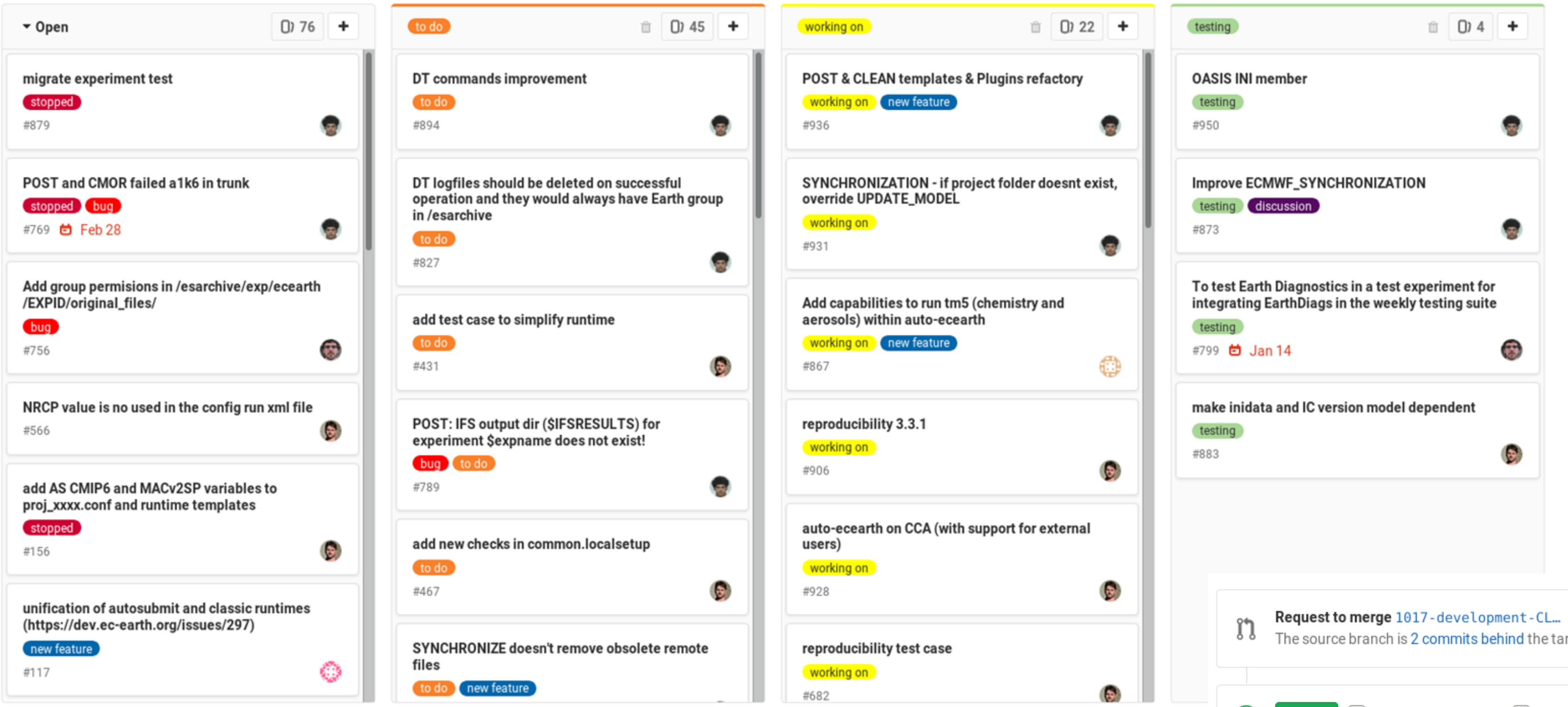
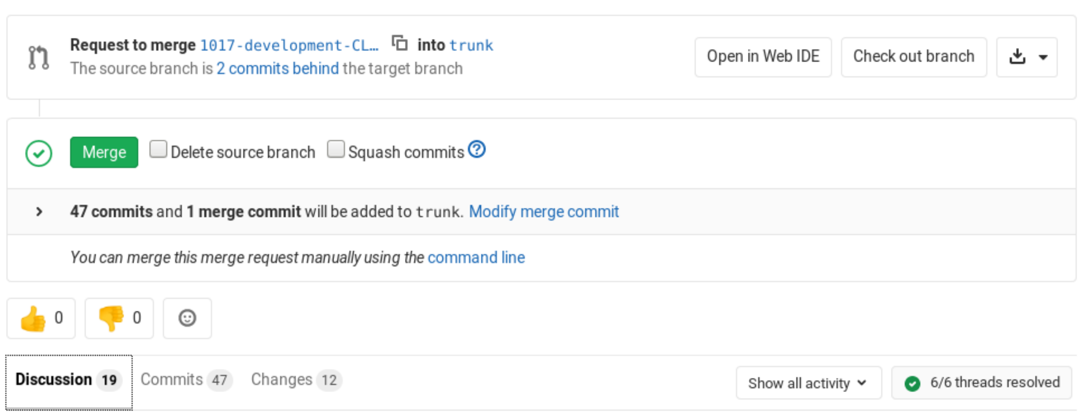
Auto-Models development



GitLab

GitLab board – Agile “Kanban” methodology

Merge requests



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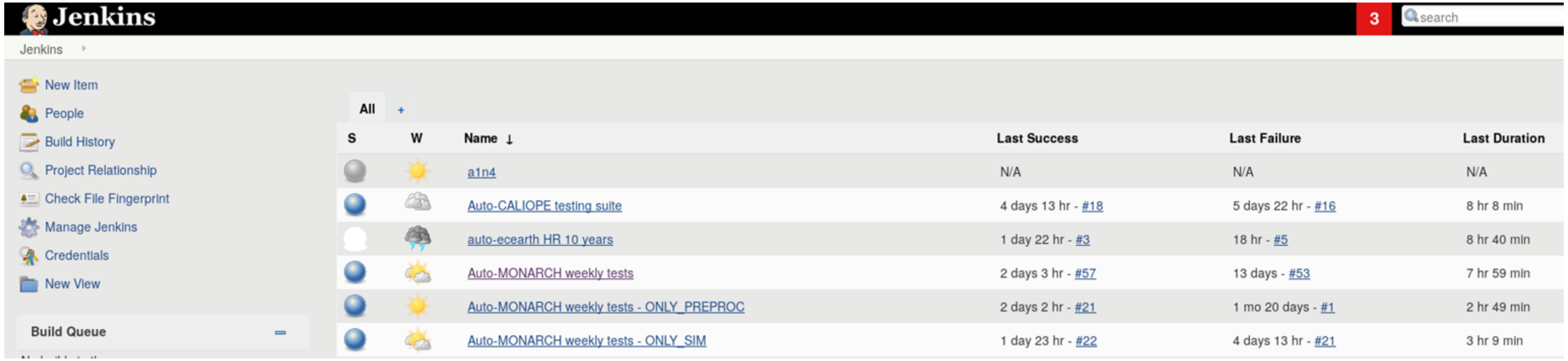
Auto-EC-Earth testing: release tests

For every version release: run a complete set of tests. Every week: run a smaller set of tests.

nord3	CCA	MN4	resolution	type	details
t02c	t00u	t00q	T255L91-ORCA1L75-LIM3	coupled	start from restart
		t00v	T255L91-ORCA1L75-LIM3	coupled	atmos. nudging
		t011	T255L91-ORCA1L75-LIM3	coupled	sppt
	t00s	t00o	T255L91-ORCA1L75-LIM3	coupled	cold start
	t01d	t00z	ORCA1L75-LIM3	nemo	cold start
		t01j	ORCA1L75-LIM3	nemo	cold start ocean nudging
	t01e	t00r	T511L91-ORCA025L75-LIM3	coupled	start from restart
		t01o	ORCA025L75-LIM3	nemo	cold start
	t01b	t00y	T511L91	ifs	cold start
	t00t	t00p	T511L91-ORCA025L75-LIM3	coupled	cold start

Integration tests: testing suite



GitLab

nord3	CCA	MN4	resolution	type	details
t02c	t00u	t00q	T255L91-ORCA1L75-LIM3	coupled	start from restart
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	t00s	t00o	T255L91-ORCA1L75-LIM3	coupled	cold start
	t01d	t00z	ORCA1L75-LIM3	nemo	cold start
		t01j	ORCA1L75-LIM3	nemo	cold start ocean nudging
	t01e	t00r	T511L91-ORCA025L75-LIM3	coupled	start from restart
		t01o	ORCA025L75-LIM3	nemo	cold start
	t01b	t00y	T511L91	ifs	cold start
	t00t	t00p	T511L91-ORCA025L75-LIM3	coupled	cold start

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AUTOSUBMIT

Reproducibility

- Earth models: variety of **spatial resolutions**, **configurations** and running **environments**.
- Scientific codes are often in a **near-constant state of development** as new science capabilities are added and requirements change.
- If we want to study the model response under some scientific changes, we have to ensure that computational **changes** do not affect the **results**.
- We need a **method** to evaluate the **computational efficiency** of our models:
  - When the hardware changes, the number of resources or the configuration changes.

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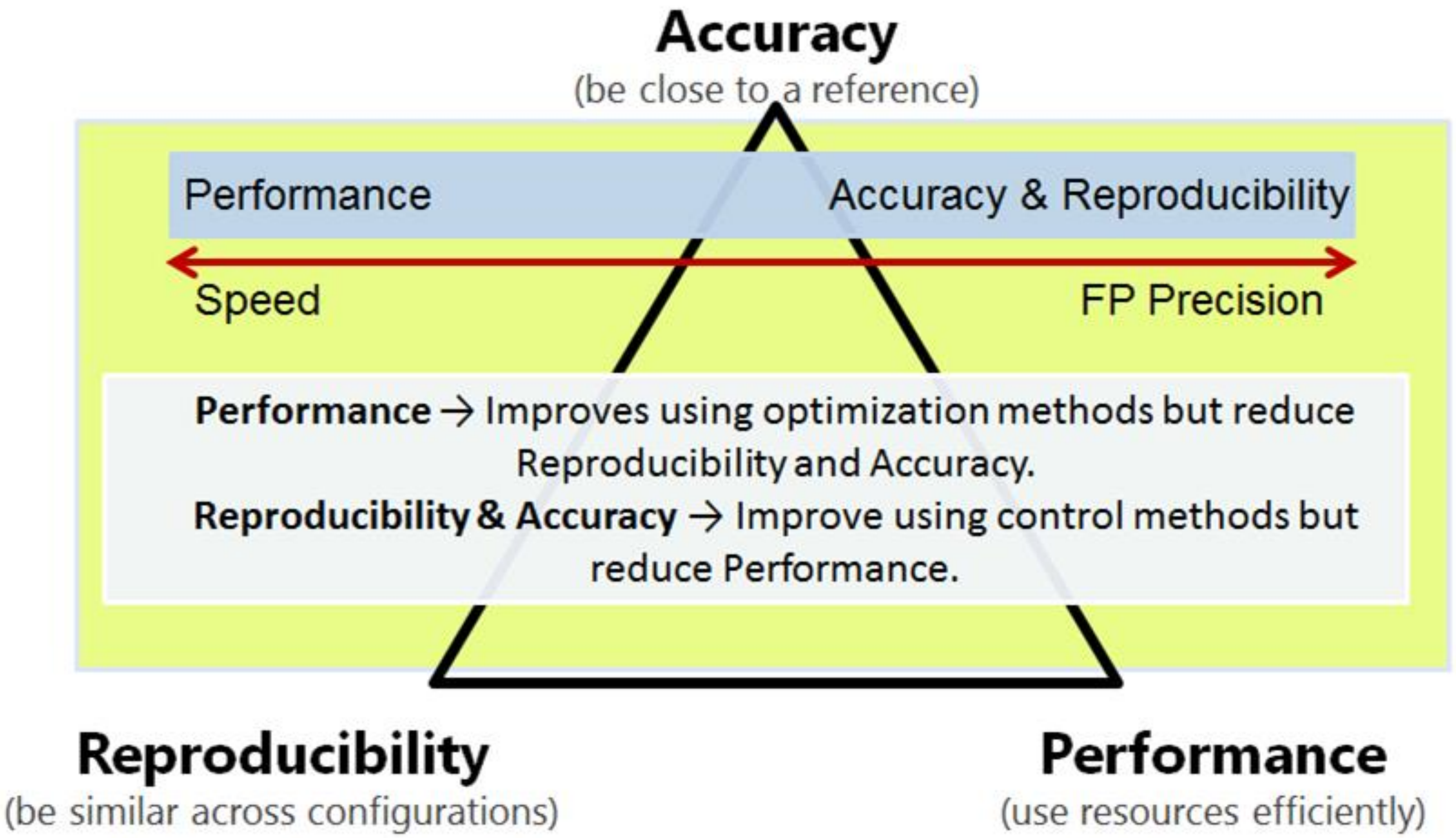
Reproducibility



Find options to control the tradeoffs among accuracy, reproducibility and performance.

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Methodology: EC-Earth CMIP6 case

20-yr long, 5-member, **Forcing Fixed**, **Cmip and Amip simulations**

Allows to look at impact of machine on mean state/bias (not possible in the case of 1-yr simulations)

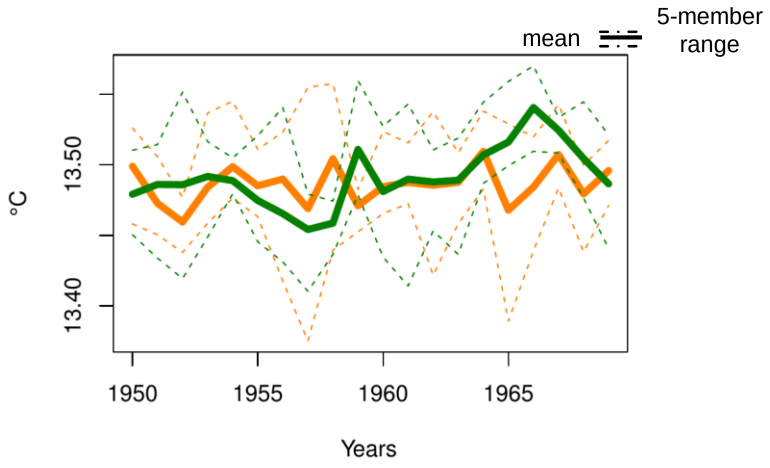
Allows to measure differences due hardware as compared to internal variability

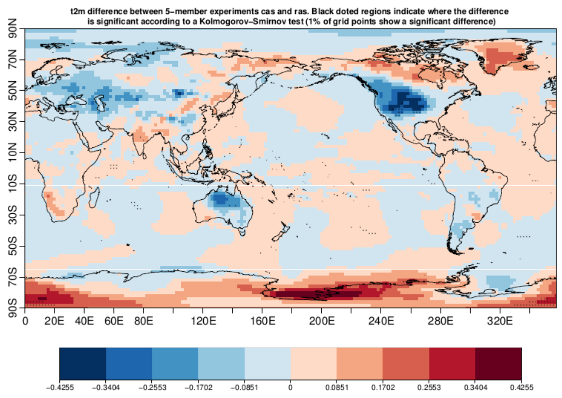
Working under stationary conditions removes possible dependence of hardware impact on the mean state

Addresses the problem from a global point-of-view; suitable to give recommendations for CMIP6

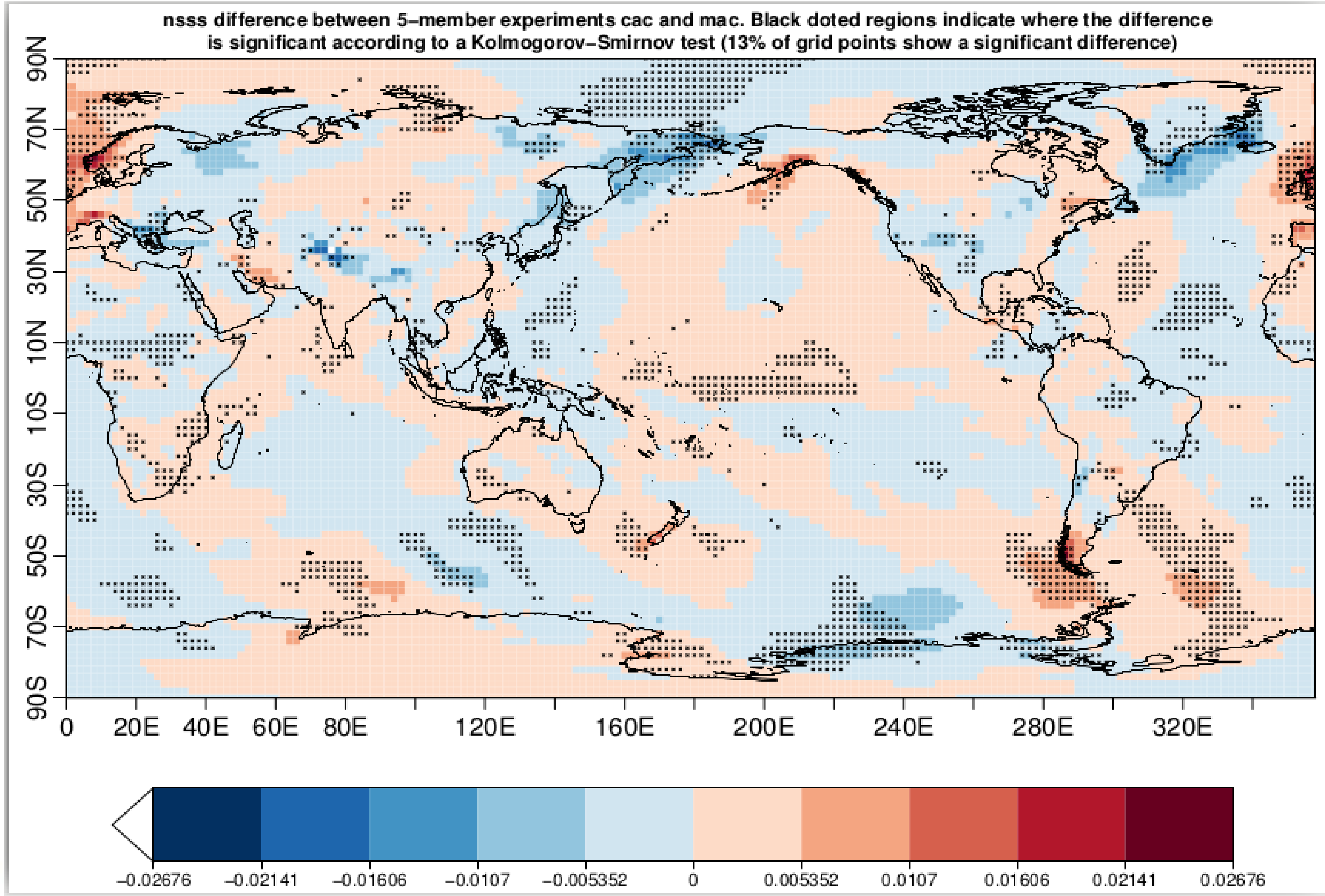
In comparison:

- Platforms
- Compilers
- Domain Decomposition
- Model options





Reproducibility: Kolmogorov-Smirnov



Methodology

Performance

- **(no-prec)**-O3 -xHost -r8 -ipo -prof-use -no-prec-div -no-prec-sqrt
- **(prof-use)**-O3 -xHost -r8 -ipo -prof-gen → -O3 -xHost -r8 -ipo -prof-use
- **(ipo)**-O3 -xHost -r8 -ipo
- **(O3)**-O3 -xHost -r8
- **(O2)**-O2 -xHost -r8
- **(no-fma_fz)**-O2 -no-fma -ftz -r8
- **(fp-except)**-O2 -fp-model except -no-fma -ftz -fpe0 -r8
- **(fp-precise)**-O2 -fp-model precise -fimf-arch-consistency=true -no-fma -fpe0 -r8
- **(fp-strict)**-O2 -fp-model strict -fimf-arch-consistency=true -no-fma -fpe0 -r8
- **(O1)**-O1 -fp-model strict -fimf-arch-consistency=true -no-fma -fpe0 -r8

Accuracy

Conclusions: EC-Earth model

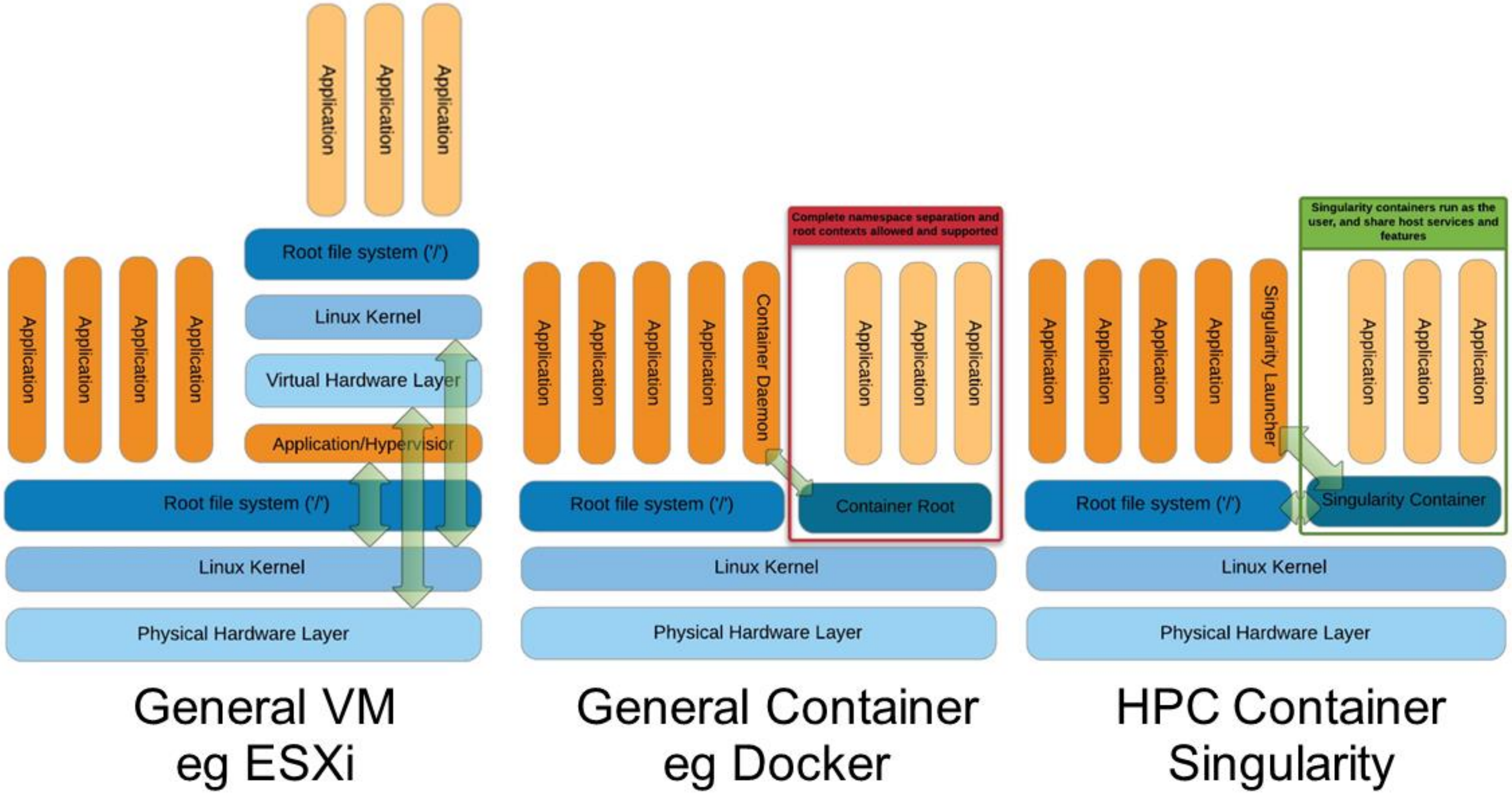
- **“Standard” flag** configurations for performance and FP precision obtain the **best results**.
  - -fp-model precise -fpe -no-fma -O2 -xHost -r8
    - Good performance, good precision, avoid fp errors, catch fpe exceptions.
  - -O2 -xHost -r8
    - Better performance (6%), good precision.
- **Aggressive optimizations** (O3, ipo, prof-use) **do not improve the performance**.
  - Some issues may avoid additional optimizations (loop dependences, non vectorization, MPI overhead …).
- **Strict FP control does not improve the precision and reduce the performance** up to 6%-12%.
- Using approximations for FP operations (no-prec-div/sqrt) do not improve the performance and reduce the precision and reproducibility dramatically.

Containerisation

- **Common recurrent problem in scientific environments**: reproducibility between different environments.

- **Containers:** make possible the virtualization at the operating system level.

Containerisation



Containerisation

- **Proposed technologies:** Singularity and Shifter, both designed to be used in HPC environments:

- **Main questions**:
  - What to containerize? The whole workflow, just the model?
  - Analyze the impact of containers within the HPC environment. ¿Computational performance?

MPMD case with singularity - Challenge: isolation level

- **Isolate** the complete **environment** is **complex** (network setup, node visibility, compiler license, etc). Then:

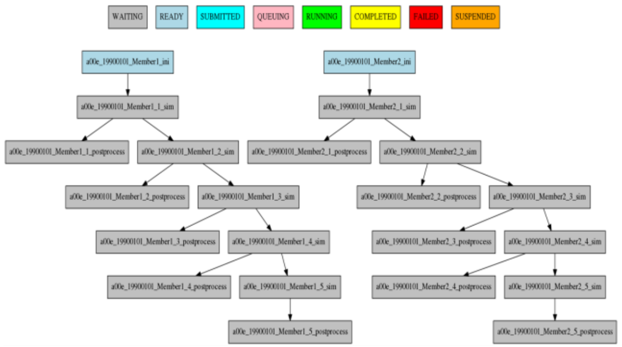
```
./mpirun  -np N singularity exec container.img exe1 :  \
                -np M singularity exec container.img exe2
```

- The executables need **binding** dynamic libraries folder and other system folders, so the call should be like:

```
mpirun  -np N singularity --bind /apps:/apps /opt:/opt /lib64:/lib64 exec container.img exe1 : \
        -np M singularity --bind /apps:/apps /opt:/opt /lib64:/lib64 exec container.img exe2...
```

Performance metrics & performance reproducibility

Climate predictions have complex workflows.
New metrics are needed to evaluate the computational efficiency.



- The simulation does **not only involve the execution of a model during a sequence of time steps** (represented by the sim job).
- The experiment **adds complexity in the horizontal for ensembles** (members with perturbations in the initial conditions).
- The experiment **adds complexity in the vertical, running long simulations** divided into chunks and including **pre- and post-processing.**

Metric	used to evaluate ...
Parallelization	Number of parallel resources allocated
Simulation Year Per Day (SYPD)	how efficient is your run job per each year of the simulation
Core-hours Per Year (CHPY)	how efficient is your run job with respect to the number of parallel resources used
Run Time (Average and Total)	how much time are per job and all the jobs in the critical path running
Queue Time (Average and Total)	how much time are per job and all the jobs in the critical path waiting in the queue
Post Run T. (Average and Total)	how much time are per job and all the jobs in the critical path running the post
Post Queue T. (Average and Total)	how much time are per job and all the jobs in the critical path waiting in the queue the post
Actual SYPD	how affect queue time to the complete experiment, from the first to the last run job
Real SYPD	How affect other issues (quota, jobs failing, rerun...) the time to complete an experiment
Energy Cost Per Year (JCPY)	how much energy is needed per each year of simulation
Data Volume	Ouput produced per year Simulated
Load Balance Cost	how much time is wasted in waiting time, produced by irregular executions

- The execution of a coupled model is complex. **Different components run in parallel**, exchanging some information and adding some extra overhead (Communication and Interpolation Time). **Load imbalances produce extra waiting time as well**.
- The execution of **each component could involve some irregular extra overhead**, such as output processing or calculations occasionally done, such as radiation.

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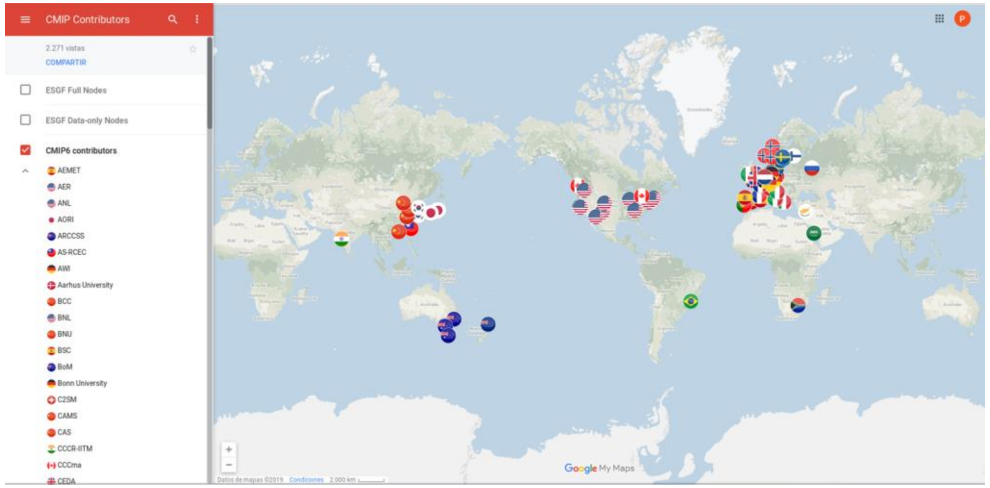
ESGF

- The **Earth System Grid Federation (ESGF)**: international collaboration serving the World Climate Research Programme's (WCRP) Coupled Model Intercomparison Project (CMIP) and supporting climate and environmental science in general.
- Web **interface** to the majority of experimental datasets used in model intercomparison projects.
- Data published have **PIDs** and **DOI**, and are heavily quality controlled.
- Data can be **discovered** and accessed through THREDDS.
- Tenths of PB of “Earth data” available.



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ESGF
Earth System Grid Federation

Some current issues

- Initial **data version control**: Need of a centralised and accessible system to share model initial data. Facilitate reproducibility and save space by incremental diff.
- Containers: Difficult to **isolate HPC environment**. Is it needed? Is it enough with statically compiled binaries?
- Model workflows are strongly based on data movement. Not so straightforward to implement **unit tests**.
- **Science reproducibility** (not b2b) still expert **human** intervention.

Thank you

The ESiWACE project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 675191

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Methodology: Reproducibility Test

- Accuracy and reproducibility
  - Reichler-Kim normalized index
    - Calculate for each variable a normalized error variance *e^2* by squaring the grid-point differences between simulated and observed climate

$$e_{vm}^2 = \sum_n \left(w_n \left(\overline{s}_{vmn} - \overline{o}_{vn} \right)^2 / \sigma_{vn}^2 \right)$$

    - Ensure that different climate variables receive similar weights when combining their errors

$$I_{vm}^2 = e_{vm}^2 \Big/ \overline{e_{vm}^2}^{\,m=20C3M}$$

    - Mean over all climate variables

$$I_m^2 = \overline{I_{vm}^2}^{\,v}$$

  - Kolmogorov-Smirnov (KS) test
    - Compare two five-member ensembles and determine whether the two ensembles are statistically indistinguishable from one another.
    - Since no prior assumption can be made on the underlying statistical distribution of the samples, the non-parametric KS test is suitable for the evaluation.

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Methodology: Reproducibility Test

- About the reproducibility methodology
  - F. Massonnet, M. Ménégoz, M.C. Acosta, X. Yepes-Arbós , E. Exarchou, F.J. Doblas-Reyes
  - https://earth.bsc.es/wiki/lib/exe/fetch.php?media=library:external:technical_memoranda:massonnet_etal_bsc-techmem-reproducibility2018.pdf
- About the reproducibility test for EC-Earth
  - Adapted by Philippe Le Sager for EC-Earth community
  - https://github.com/plesager/ece3-postproc#reproducibility-test
- About the reproducibility results and how to collaborate
  - Contact Mario (mario.acosta@bsc.es) and Philippe (sager@knmi.nl)
  - Provide feedback: https://dev.ec-earth.org/issues/533
  - People collaborating: Uwe Fladrich (SMHI), Jose M. Rodríguez (AEMET), Paul Nolan (ICHEC)

Methodology: CPMIP Metrics

- About the CPMIP Metrics
  - V. Balaji et al. 2017
  - https://www.geosci-model-dev.net/10/19/2017/gmd-10-19-2017.pdf
- About the adaptation for EC-Earth
  - Adapted by Uwe Fladrich and Domingo Manubens for EC-Earth
  - Adapted by Philippe Le Sager for common CCA (ECMWF) experiments
  - Adapted and extended by Mario Acosta and Domingo Manubens for MN4 (BSC) using a workflow manager
- About future plans
  - Improvement and Portability of CPMIP metrics for ESMs in IS-ENES3 (Mario Acosta, Eric Maissonaive…).
  - Work in collaboration with the community (V. Balaji, Pier-Luigi…)
- About the CPMIP results and how to collaborate for CMIP6 runs
  - Contact Mario (mario.acosta@bsc.es) and Philippe (sager@knmi.nl)
  - Provide feedback: https://dev.ec-earth.org/issues/532
  - People collaborating: Uwe Fladrich (SMHI), Jose M. Rodríguez (AEMET), Paul Nolan (ICHEC)

- What it is:
  - https://esgf-node.llnl.gov/search/esgf-llnl/
  - web portal to download climate (CMIP5-6, SPECS, obs4MIPS, CORDEX,...) data
  - ingests very standardized data (CMOR-$proj)
- There are data nodes and index nodes:

  https://www.google.com/maps/d/u/0/viewer?mid=1qgItlbd11j6wzirf6vo2Zq_uYqaP4baQ&ll=43.83402373129155%2C14.074149978563128&z=4

  - Data nodes **host the data** and have a thredds server displaying the data hosted locally
  - https://esgf.bsc.es/thredds/catalog/catalog.html
  - Indexes have a landing page allowing to search