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Workshop on workflows Brussels, 13 September 2018



Barcelona Supercomputing Center Centro Nacional de Supercomputación

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From Autosubmit to Cylc

A community standard for the EC-Earth consortium?

Domingo Manubens



We conducted a survey among the EC-Earth community to know about their use cases and asking about their needs and expectations from a workflow management system.

Participants: 34
 (12 countries / 18 institutions)

Country	Institution	# participants
Sweden	Lund (3), SU (2), SMHI (2)	7
Spain	BSC	6
Netherlands	KNMI (3), NSC (1), IMAU(1)	5
Finland	FMI (3), CSC (1)	4
Belgium	UCL	3
Germany	AWI (1), KIT (1)	2
Denmark	DMI	2
Italy	ENEA	1
Norway	UiB	1
Portugal	UL	1
United Kingdom	University of Oxford	1
Ireland	ICHEC	1

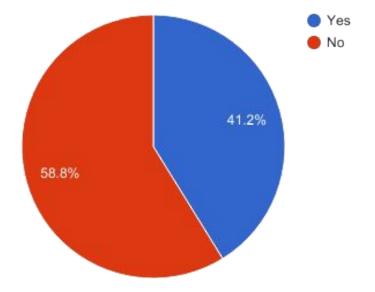
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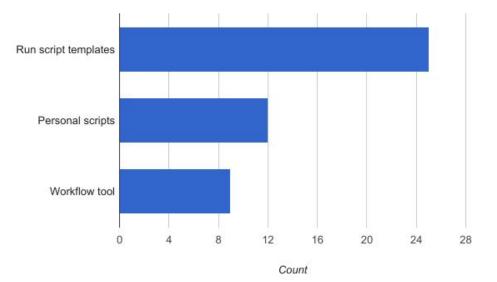




Have you used a workflow management system?





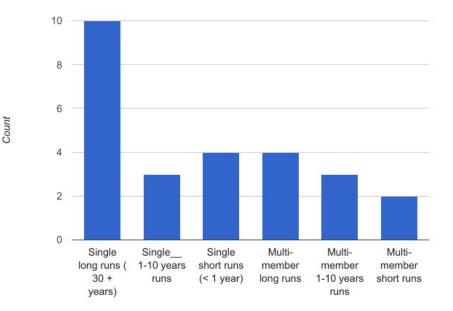


How do you run -**EC-Earth?**

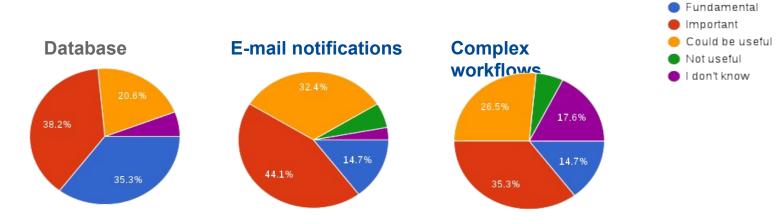


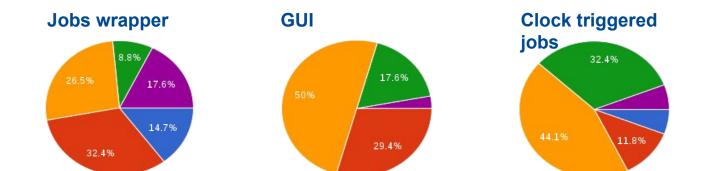
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Model simulation _ production



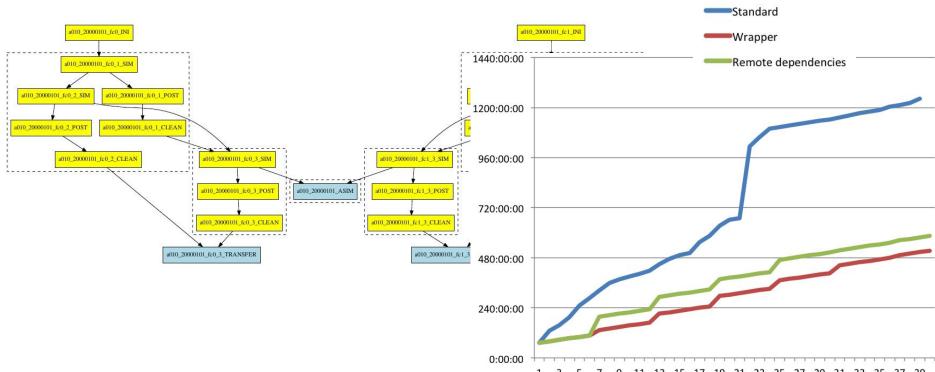






Autosubmit wrappers (job clustering)

different jobs together.



Motivation: to **improve** the throughput by **reducing** queueing **time** by wrapping

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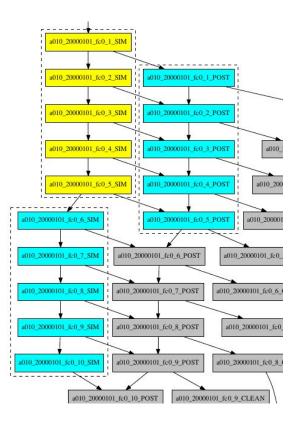
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Vertical wrapper

- The status of each job is checked and updated
- Failures are detected, also when a job is running for longer than its wallclock
- In this case, the whole wrapper job is cancelled, and, if there are retrials, resubmitted from the point of failure

[wrapper]
TYPE = vertical
JOBS_IN_WRAPPER = SIM POST



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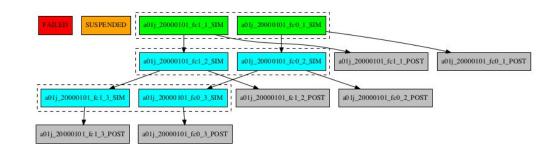
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Horizontal wrapper

• Usage of machinefiles in mpirun identified by the job name

[wrapper] TYPE = horizontal JOBS IN WRAPPER = SIM POST



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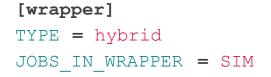
BSC

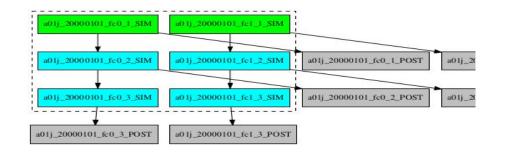
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Hybrid wrapper

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- Mix of vertical and horizontal wrappers
- Runs in parallel independent members, each one having a sequence of jobs that depend on one another

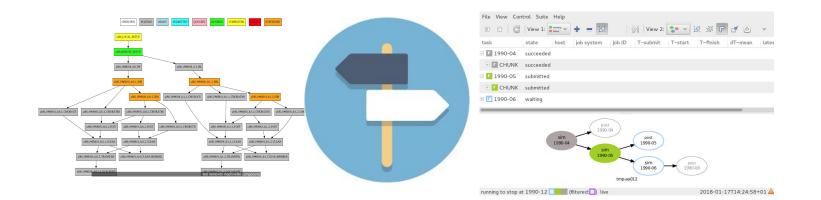




From Autosubmit to Cylc

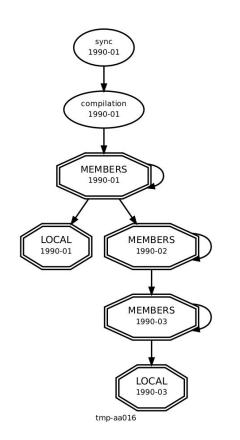


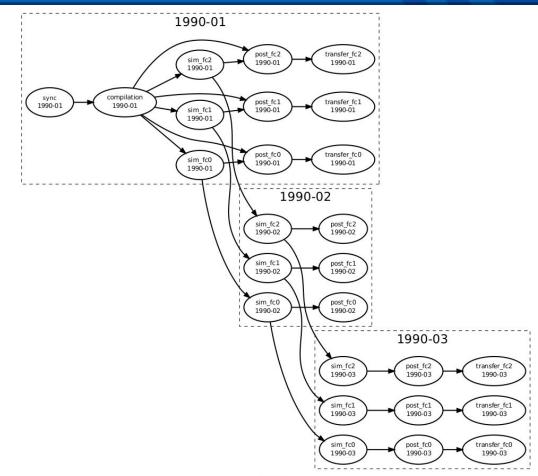
- Some people are interested in a workflow management system common for EC-Earth
- Option Autosubmit is available and will be maintained
- Option Cylc will be implemented in the next 1-2 years



Cylc - workflow engine







tmn-aa016

Rose - configuration management, GUI

Goal: to facilitate suite development, management and collaboration

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Rosie - experiment database



Goal: version controlling suites and suite discovery and management

mp: Rosie Su	uites Discovery	@ bscearth200								search query
Search term	a	l revisions search								
detail 🔺	idx (branch 🕴	revision 🔶	owner	project 🔶	title \$	author 🔶	date 🎍	from_idx	status
I	tmp-aa000	trunk	2	dmanuben	specs	test	eadmin	2017-10-18T08:29:22Z	None	A
I	tmp-aa001	trunk	3	dmanuben	tmp	tmp1	eadmin	2017-11-27T12:25:58Z	None	A
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I	tmp-aa006	trunk	8	dmanuben	primavera2	spinup	eadmin	2017-11-28T09:39:04Z	tmp-aa004	А
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EC-Earth runtime

Basic set of portable runscript templates

- Classic
 - Simulation template for 4 use cases (ESM, GCM, IFS only, NEMO only) single runs, multiple platforms supported
 - Variable definitions on templates can be overwritten with specific parameters from config-run.xml at runtime
- Autosubmit
 - The same but support for taking parameters from Autosubmit config files

subversion / ecearth3 / trunk

Name	Size	Revision
+ 🖿 doc		5483
- 🖕 runtime		5800
+ 🖿 autosubmit		5800
- 🖕 classic		5799
+ 🖿 ctrl		5747
+ 🖿 platform		5788
a config-run.xml	9.03 KB	5312
C ece-esm.sh.tmpl	50.2 KB	5799
C ece-ifs+nemo.sh.tmpl	32.5 KB	5799
C ece-ifs.sh.tmpl	22 KB	5799
C ece-lsm.sh.tmpl	20.1 KB	5583
🗅 ece-nemo.sh.tmpl	22 KB	5490
librunscript.sh	7.47 KB	3977
libsave_ic.sh	19 KB	5483
+ 🖿 datacheck		5747
+ 🖿 sources		5788

5

EC-Earth Cylc runtime

- Same idea as for Autosubmit runtime
 - Config-run.xml parameters can be taken from a rose-app.conf

suite info suite conf copy-runtime command	Environment variab	le configuration
copy-runtime		
	CHPCHOST	
command		mnl.bsc.es
env	C HPCROOTDIR	/gpfs/scratch/bsc32/bsc32704/tmp-aa012
Stress)	IPCUSER	bsc32704
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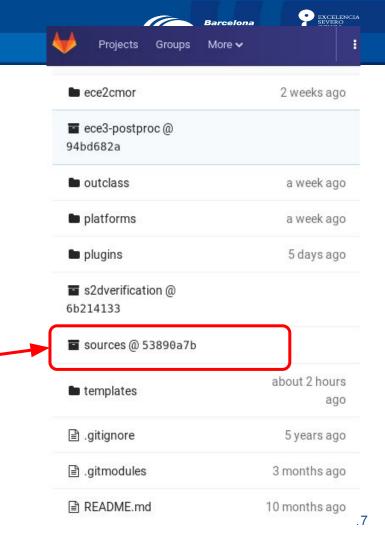
EC-Earth 3

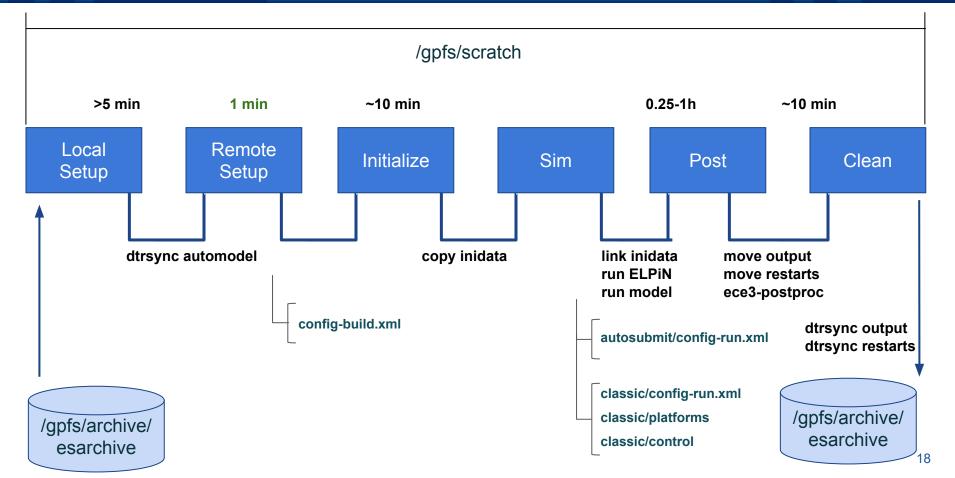
subversion / ecearth3 / branches / development / 2018 / r4871cylc-runtime

Name	Size	Revision
+ 🖿 doc		5328
- 🖕 runtime		5449
+ 🖿 autosubmit		5449
+ 🖿 classic		5449
─ 🖕 cylc		5449
Compilation.sh	7 KB	5449
i config-run.xml	9.35 KB	5449
🗋 ece-esm.sh.tmpl	48.7 KB	5449
C ece-ifs+nemo.sh.tmpl	31.1 KB	5449
ece-ifs.sh.tmpl	20.8 KB	5449
🕒 ece-lsm.sh.tmpl	18.2 KB	5449
🗋 ece-nemo.sh.tmpl	20.3 KB	5449
🖹 sync.sh	838 Bytes	5449
+ 🖿 datacheck		5328
+ 🖿 sources		5328

Auto-EC-Earth

- Framework to run EC-Earth versions with Autosubmit smoothly
 - BSC-ES additional tasks templates (setup, compilation, transfer ...), support for seasonal runs and more complex use cases (data assim, diagnostics, jobs wrapper...) are provided on a different repository (git)
 - It includes EC-Earth basic runtime as Git submodule
 - All BSC-ES production and development experiments start from an Auto-EC-Earth branch or tag





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Auto-EC-Earth, set of tests



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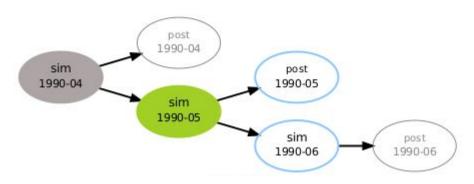
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		t011	T255L91-ORCA1L75-LIM3	coupled	sppt	
	t00s	t00o	T255L91-ORCA1L75-LIM3	coupled	cold start	
	t01d	t00z	ORCA1L75-LIM3	nemo	cold start	
		t01j	ORCA1L75-LIM3	nemo	cold start ocean nudging	
	t01e	t00r	T511L91-ORCA025L75-LIM3	coupled	start from restart	
		t01o	ORCA025L75-LIM3	nemo	cold start	
	t01b	t00y	T511L91	ifs	cold start	
	t00t	t00p	T511L91-ORCA025L75-LIM3	coupled	cold start 19	

Cylc adoption at BSC (WIP)

- Climate prediction
 - EC-Earth / NEMO / OpenIFS
 - Historical runs
 - Seasonal / decadal runs
 - Model development (stem?)
- Air quality
 - MONARCH
 - Operational runs
- Computational group
 - Automated tests on multiple platforms
 - Scalability analysis
 - Load balance analysis
 - Precision analysis
 - Data provisioning

Portable experiments including

- Compilation
 - Initialization
- Simulation
 - Post processing
 - Automated transfers
 - Data assimilation





Ongoing work

- Barcelona Supercomputing Center Centro Nacional de Supercomputación
- Portable suites for collaborative model development
 - EC-Earth Cylc runtime simplification
 - Rose metadata compliance
 - Rose stem, is it useful in the testing/development phase?
 - Rosie web services under EC-Earth Development portal
- Capture more use cases @ BSC
 - Suite for ensemble climate prediction
 - Suite for ensemble MONARCH (operational air quality model)
 - System wide installation of Cylc and Rose
- Cylc @ MN4
 - Communication back from tasks to suite host will be possible



- Cylc @ ECMWF
 - Rose suite running at ECMWF, including tasks to archive data at BSC and compute diagnostics on Power9 cluster
 - Will Cylc web-based GUIs be available from ECMWF servers?
 - Could ECMWF HPC be used as remote resource, using the ecaccess web toolkit?
- (later) Single batch job for multiple tasks #2754





- A strategy for adopting Cylc and Rose as the EC-Earth common workflow management system is being build
 - Needs of the community have been taken into account
- A demonstrator has been created at BSC
 - Cylc, Rose and Rosie have been installed on a private virtual machine at BSC
 - Rose suites have been created for running EC-Earth historical and multi-member ensemble climate simulations
 - MareNostrum 4 (Slurm) and data-transfer nodes (background) are being used as remote resources, using polling

Next steps



- EC-Earth consortium collaboration
 - Develop more EC-Earth use cases
- Close collaboration with the MetOffice
 - ESiWACE 2
 - IS-ENES 3
- Training activities
 - Cylc + Rose from scratch, suite design, at BSC
 - Tutorials at EC-Earth meeting and PATC course







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Thank you!

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