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# EasyBuild site presentation: BSC Earth Sciences

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Computational Earth Sciences

25/01/2022

7th EasyBuild User Meeting

# Outline

- Who we are?
- Why using EasyBuild?
- Integration of EasyBuild in Earth Sciences workflow
- Next steps

# Disclaimer



## Disclaimer

This presentation is based on **Earth Sciences experience**, a research department from Barcelona Supercomputing Center.

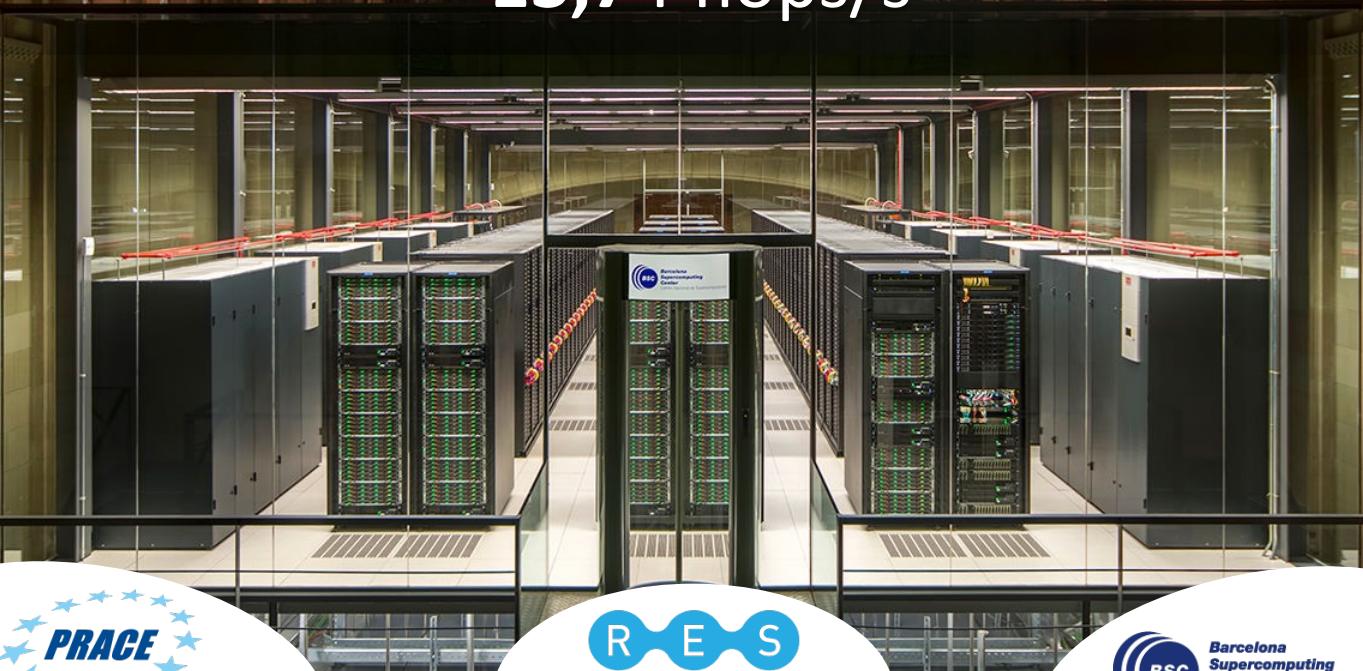
It does **not reflect any view or strategy from the Operations** department, managers of the Mare Nostrum 4 (an other HPC).

This is a **user presentation**.

# The MareNostrum 4 supercomputer

Total peak performance:

**13,7 Pflops/s**



Access: [prace-ri.eu/hpc-access](http://prace-ri.eu/hpc-access)



RED ESPAÑOLA DE  
SUPERCOMPUTACIÓN

Access: [bsc.es/res-intranet](http://bsc.es/res-intranet)

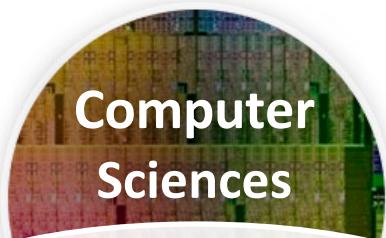


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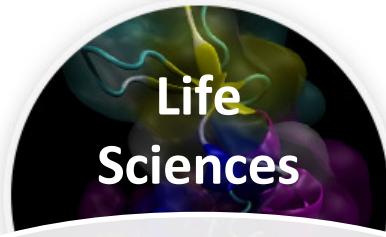


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# Mission of BSC Scientific Departments



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



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



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



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

# BSC Earth Sciences

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



## Service Users Sectors



Infrastructures



Solar Energy



Urban development



Transport



Wind Energy



Agriculture



Insurance

# Why using EasyBuild?

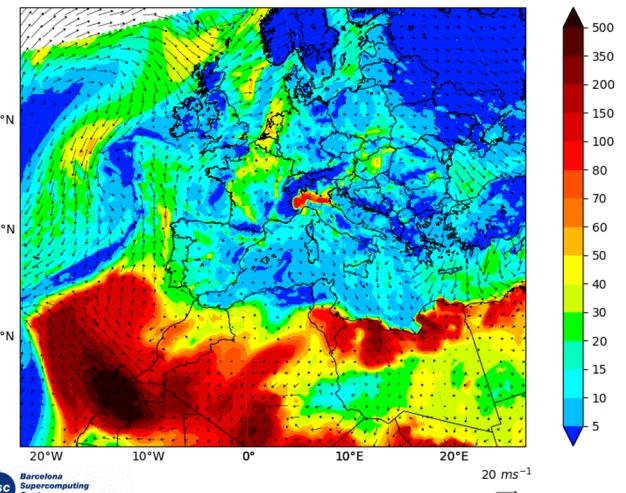
Workstations



Virtual Machines

HPC's

PM10 ( $\mu\text{g m}^{-3}$ ) for 00UTC 16 Jan 2022  
BSC-ES/FORECAST CALIOPE - Resolution: 12 km x 12 km



# Functionalities

- **Reusability:** users can develop on workstations and run in HPC
- **Stability:** operational forecasting needs a freezed environment → (i.e. python packages)
- **Reproducibility:** clear picture of the environment used to produce data
- **Deployment:** reduced time when entering in a new cluster
- **Flexibility:** different architectures (including Cloud) and improved migration (machine with updated OS)
- **Community:** reuse and share easy-configs

# Current EB installations

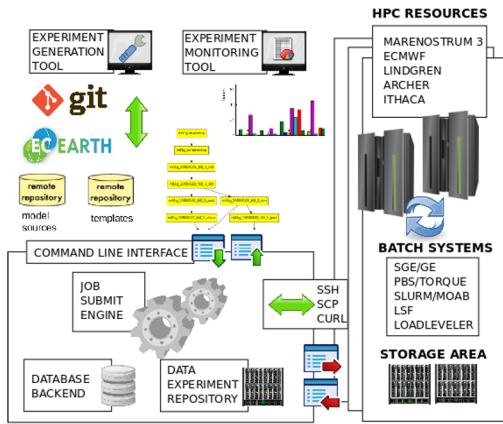
- Workstations and VMs
  - Production: foss-2015a
  - Pre-production (stopped): foss-2019b
- HPC
  - Nord3: foss-2019b
  - Power 9: foss-2018b and fosscuda-2019b
  - Cirrus (Spanish Meteorological Agency): foss-2020a
- Cloud
  - Huawei: foss-2019b
  - Oracle: foss-2019b

```
[bsc32353@login4 /gpfs/projects/bsc32/software]$ tree -L 3
.
├── rhel
│   ├── 7.4
│   │   '-- ppc64le
│   '-- 7.5 --> 7.4
└── suselinux
    '-- 11
        '-- x86_64
```

Hierarchichal structure for HPC modules

# The workflow manager

**AUTOSUBMIT**



## Automatization

- Dependency based
- Meta-scheduler
- Multi-platform
- Auto retries

## Efficiency

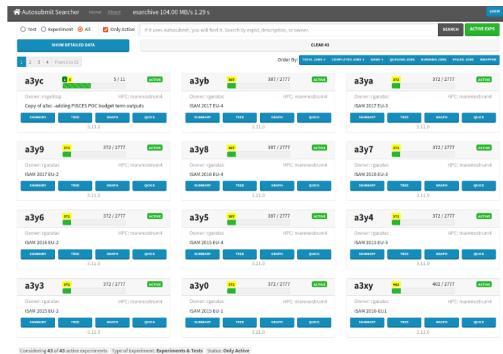
- Job packages
- Presubmission

## Monitorization

- Plots
- Statistics
- Experiment ddbb

## Tools

- Migrate exp.
- Archive exp.



Autosubmit web GUI

## Accessibility

- Web based
- Advanced search

## Monitorization

- Different views
- Real time updates

## Analysis

- Job log files
- Stats and metrics
- Cost estimation

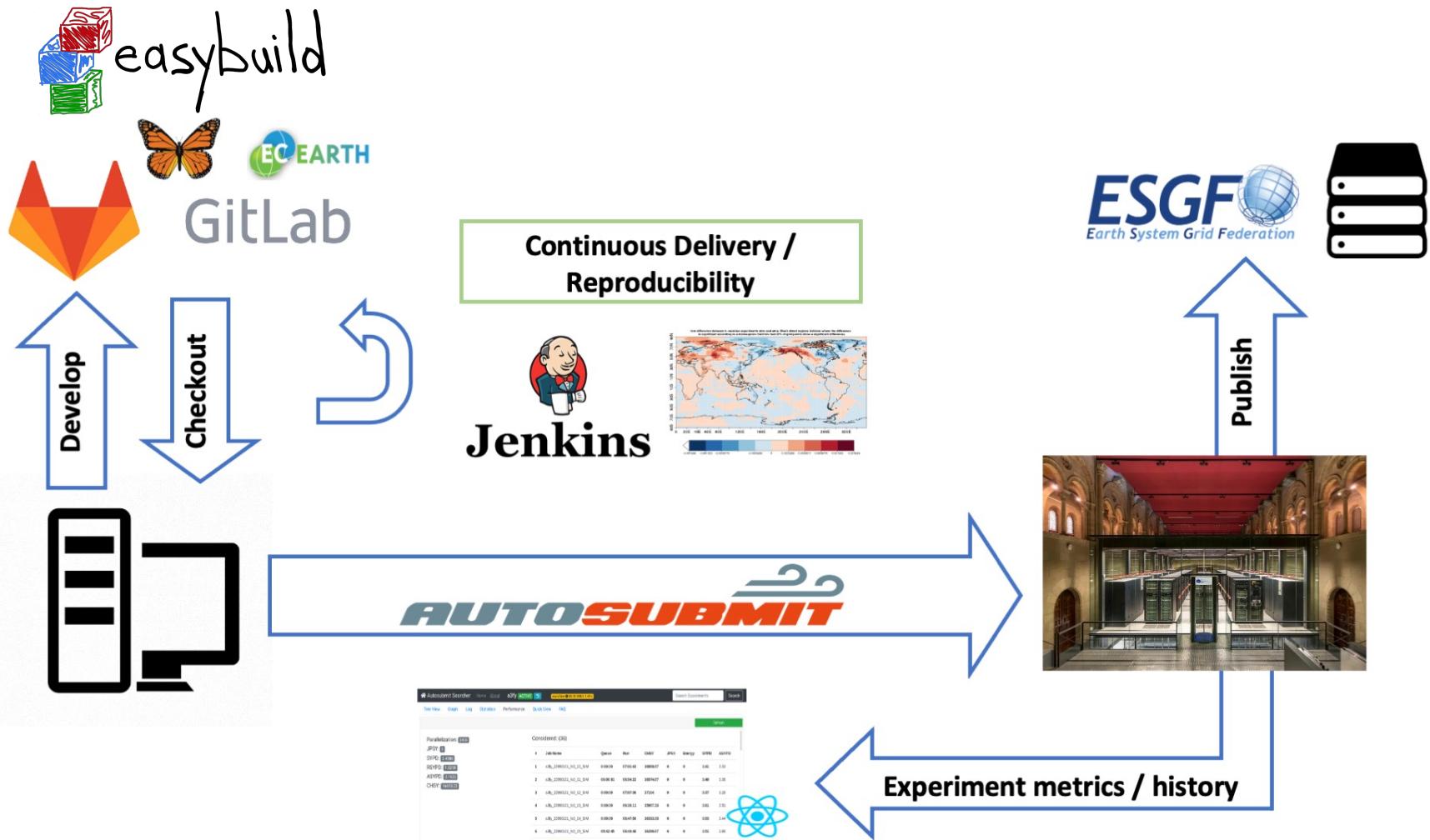
## Management

- Authentication
- Exp. management

D. Manubens-Gil, J. Vegas-Regidor, C. Prodhomme, O. Mula-Valls and F. J. Doblas-Reyes, (2016). "Seamless management of ensemble climate prediction experiments on HPC platforms", 2016 International Conference on High Performance Computing & Simulation (HPCS), Innsbruck, pp. 895-900. <https://doi.org/10.1109/HPCS.2016.7568429>

W. Uruchi, M. Castrillo and D. Beltrán, (2021). "Autosubmit GUI: A Javascript-based Graphical User Interface to Monitor Experiments Workflow Execution", Journal of Open Source Software, 6(59), 3049. <https://doi.org/10.21105/joss.03049>

# Model workflow

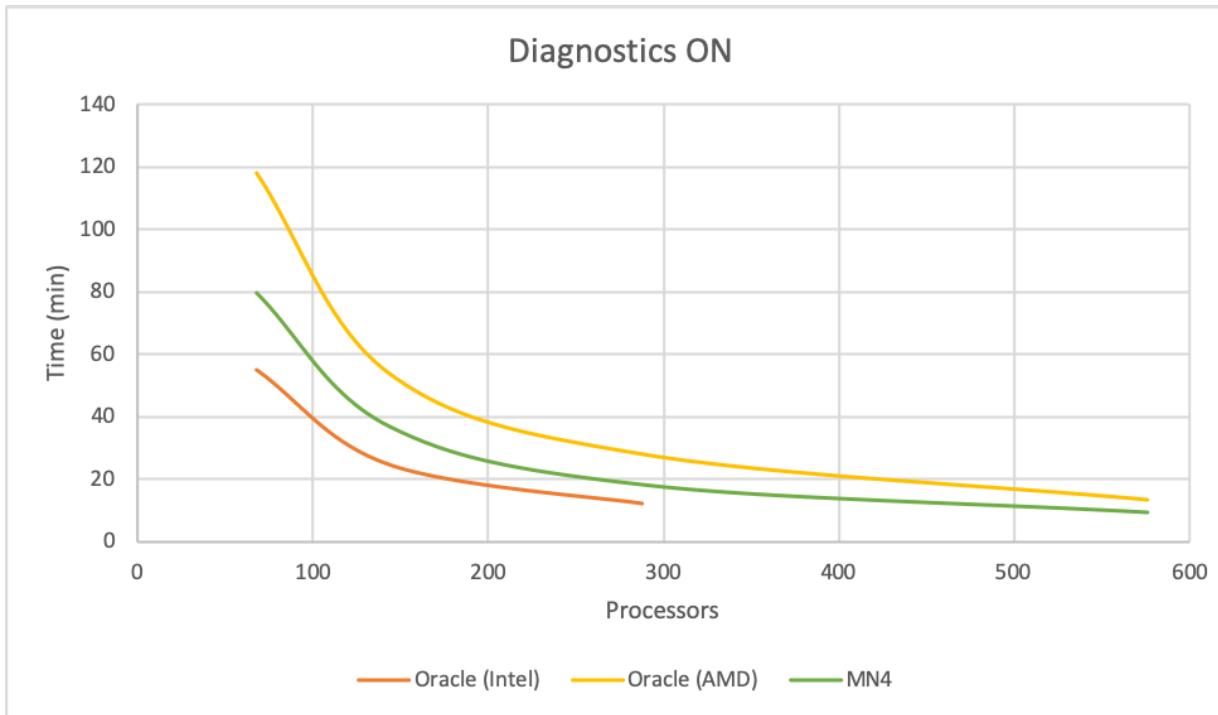


# Enhancing deployments

- Steps to deploy our forecasts in a new machine
  - Access the machine
  - Deploy EB
  - Deploy our usual software stack
    - GCC, OpenMPI, netCDFs, ESMF... (and dependencies)
    - Python and R (+ packages)
  - Deploy our workflow manager (Autosubmit)
  - Deploy auto-model (templates with modules)
  - Run the model
- Last year, MONARCH atmospheric chemistry model was running in AEMET new cluster (cirrus) in **less than two weeks** (with minimal interaction with local sysadmins)

# EasyBuild in the Cloud

- In 2021, in collaboration with HPCNow!, we did a Proof Of Concept (PoC) using ORACLE Cloud to port our atmospheric chemistry workflow to the Cloud (BSC is not a 24/7 site)



# What we need to improve

- Update toolchains
- Purging old modules
- Sharing developed custom easy-configs
- Involvement in EasyBuild community

# Next steps

- Update some of our toolchains
- Continue to use EB as software deployment tool



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# Thank you

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