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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.

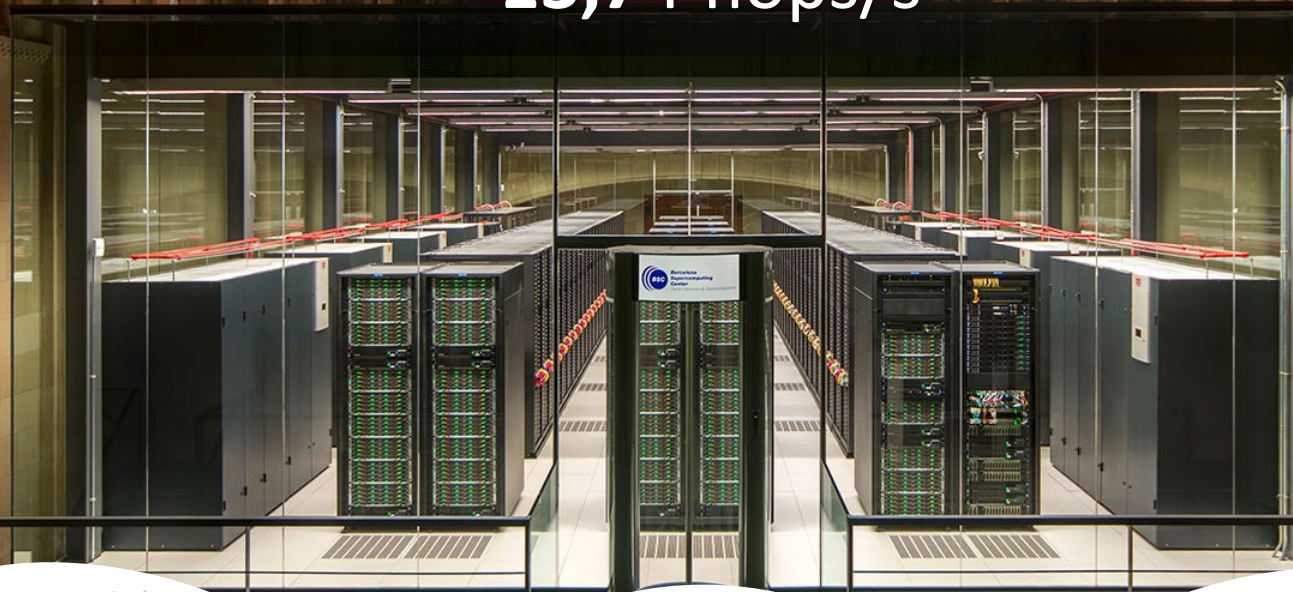
It does **not reflect any view or strategy from the Operations** department, managers of the Mare Nostrum 4 (an other HPC).

This is a **user presentation**.

The MareNostrum 4 supercomputer

Total peak performance:

13,7 Pflops/s



Access: prace-ri.eu/hpc-access



RED ESPAÑOLA DE
SUPERCOMPUTACIÓN

Access: bsc.es/res-intranet



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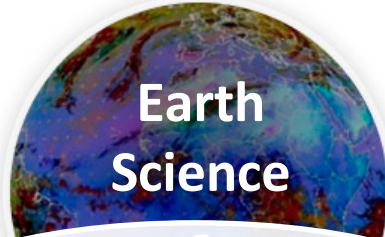
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Mission of BSC Scientific Departments



Computer Sciences

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



Earth Science

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



Life Sciences

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

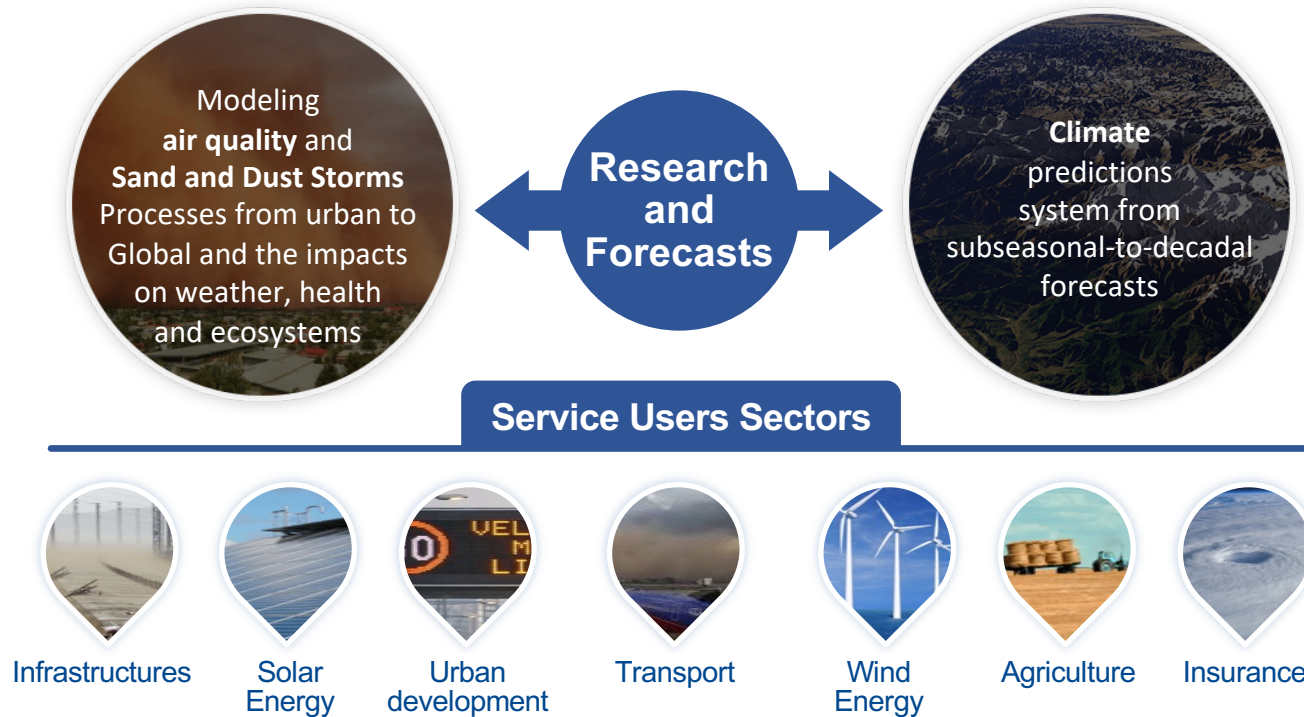


CASE

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

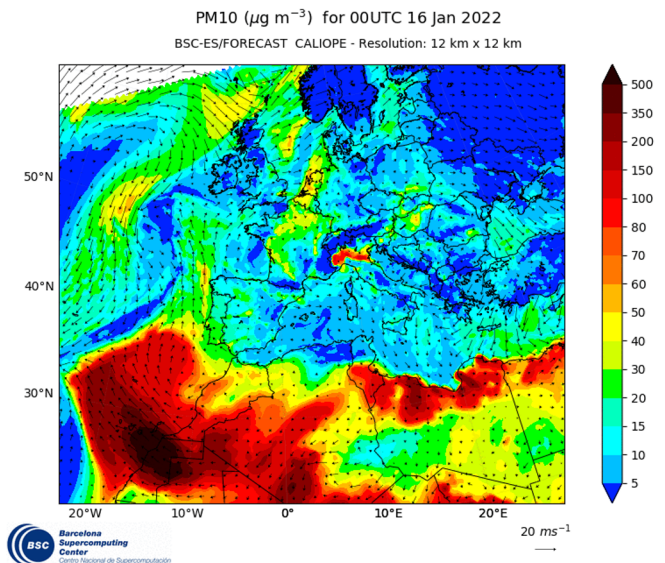


Why using EasyBuild?

Workstations

Virtual Machines

HPC's



Functionalities

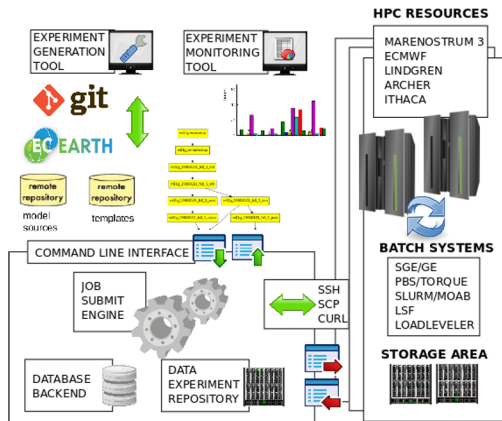
- **Reusability:** users can develop on workstations and run in HPC
- **Stability:** operational forecasting needs a freezed environment → (i.e. python packages)
- **Reproducibility:** clear picture of the environment used to produce data
- **Deployment:** reduced time when entering in a new cluster
- **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
|   |-- 7.5 -> 7.4
|-- suselinux
|   |-- 11
|   |-- x86_64
```

The workflow manager **AUTOSUBMIT**



Automatization

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

Efficiency

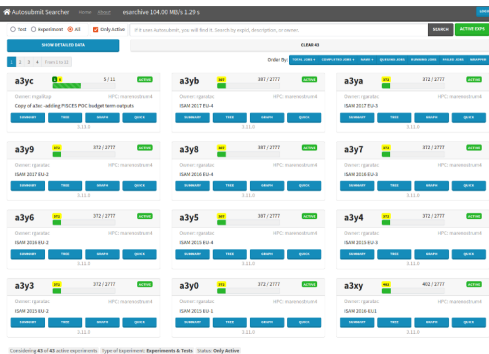
- Job packages
- Presubmission

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

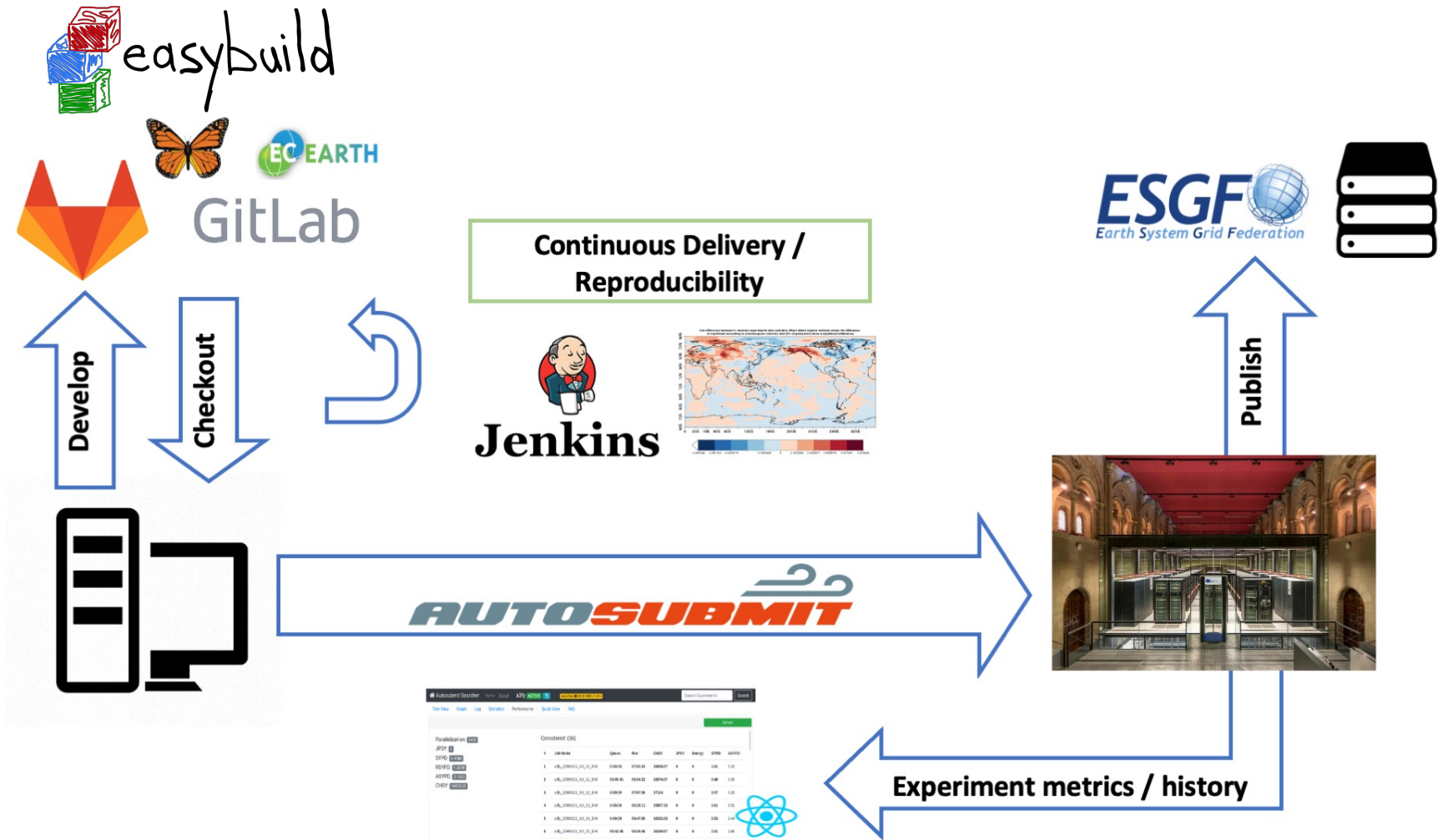
Management

- 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/HPCSim.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

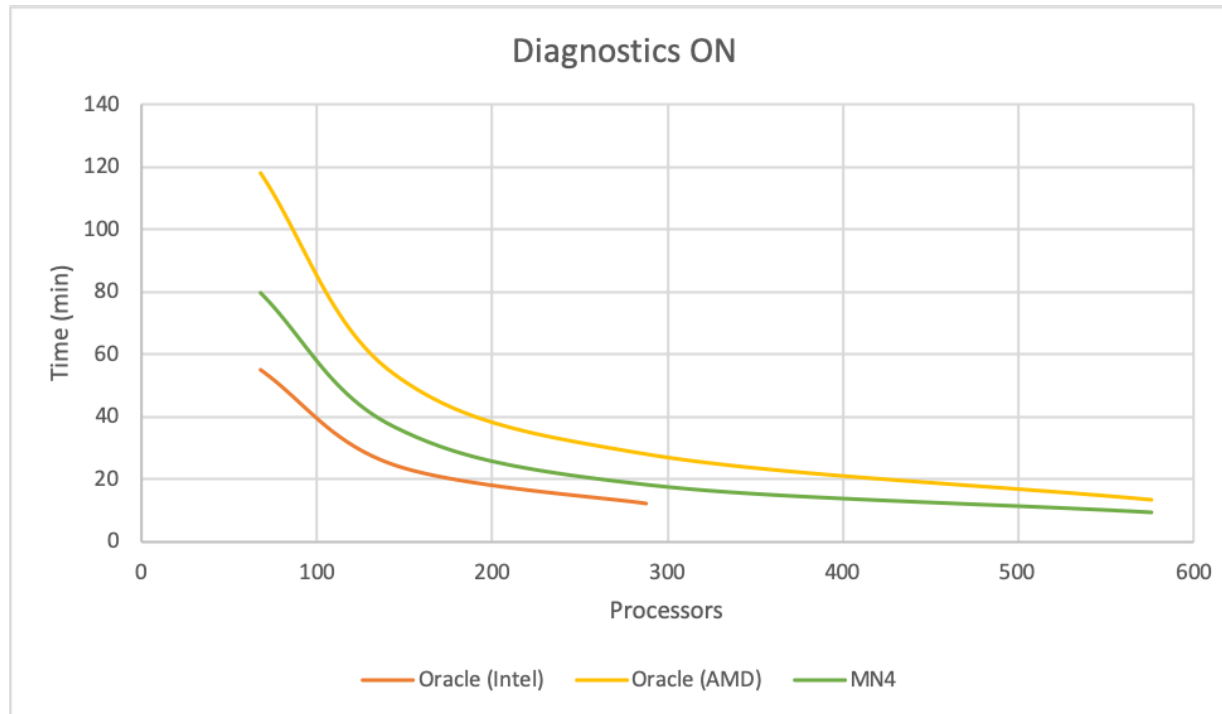


Enhancing deployments

- 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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