GAIA : Software deployment through CI
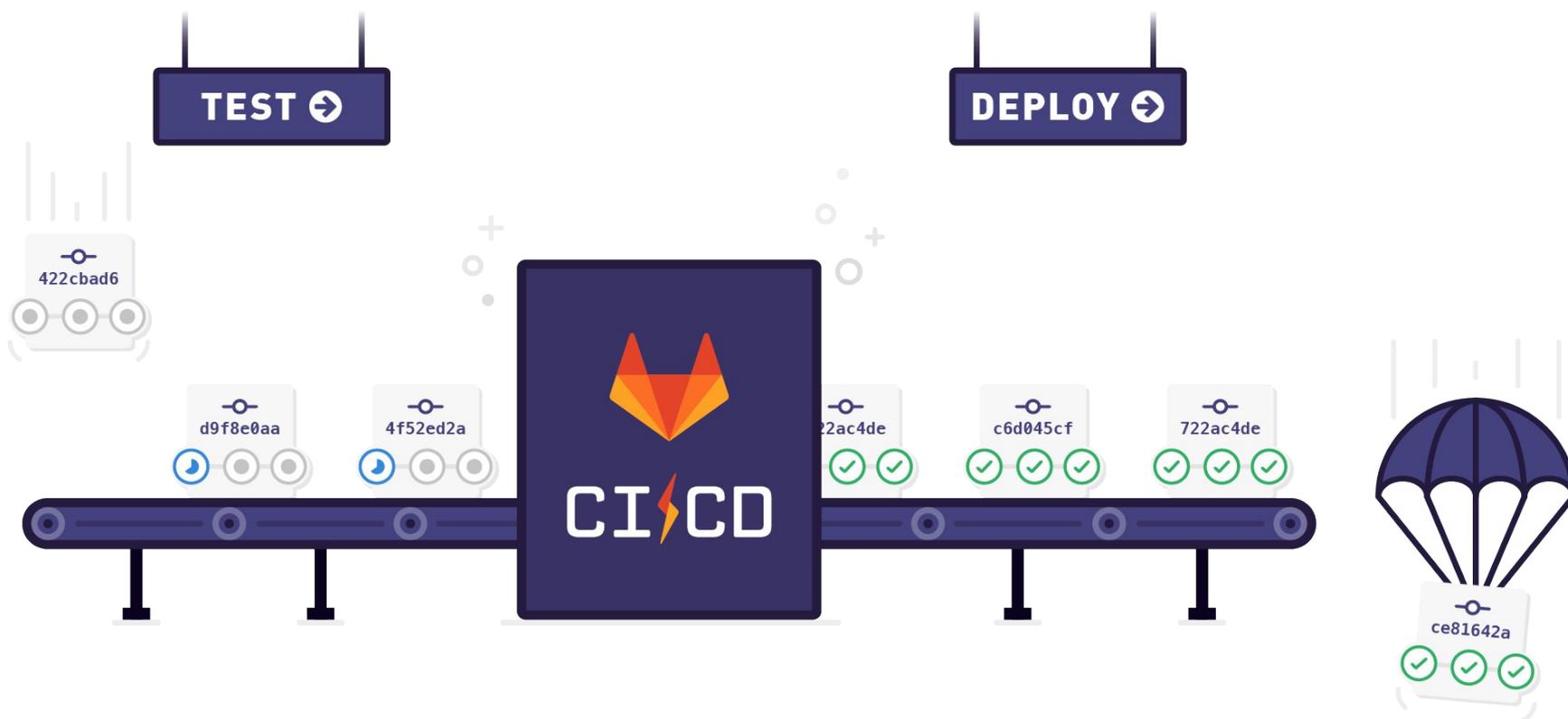
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- # Objectives

  - ➢ Automate **software deployment** and module generation.
  - ➢ Automate **validation and testing** of functionality and performance.
  - ➢ Deployment **reproducibility**

- # Project Overview In Figures

The Gaia project, initiated in 2019 on OCCIGEN, now manages all software stacks for ADASTRA.
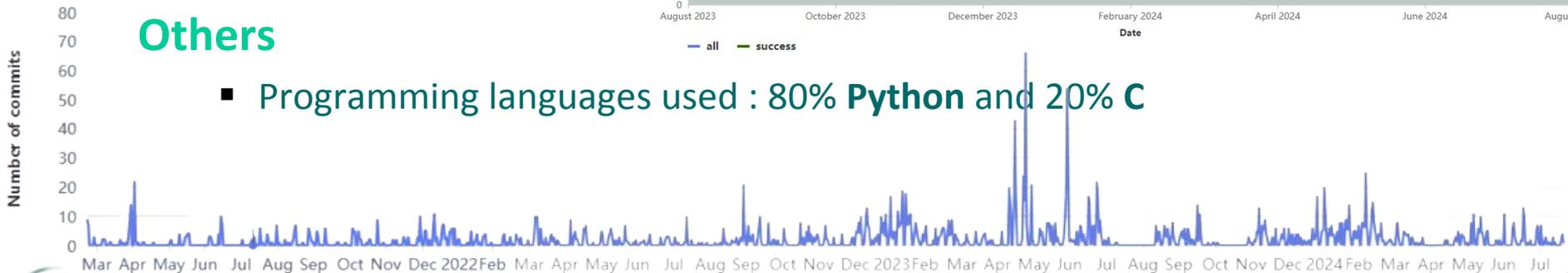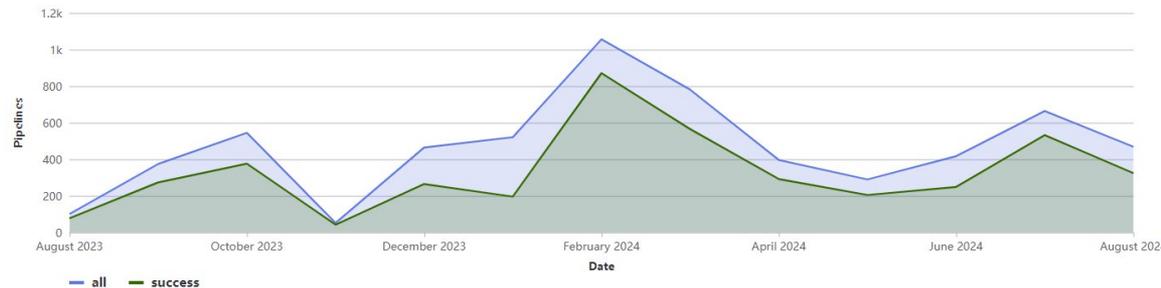
Commit statistics

- Total: 2000 commits
- Average per day: 2.4 commits
- Authors: ~ 15

CI/CD Analytics

- Total Pipelines: 4041
- Success ratio: 52.84%
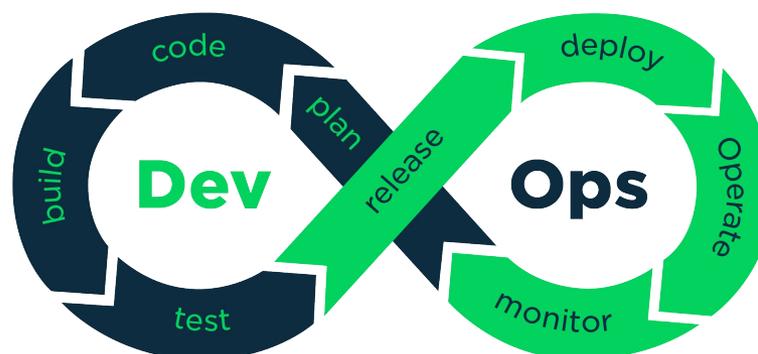
Others

- Programming languages used : 80% **Python** and 20% **C**

- # Generality :

How we work ?

- Issues, branch, merge request (Milestone and Sprint)
- DevOps:

Which tools ?

- **Gitlab :** Collaborative tools for **Code Repository** and **CI/CD**
- **Spack :** Software deployment tool : **Packages** and **Modules**
- **Reframe :** Framework for writing regression tests

• **Gitlab**

- CINES Internal repository: <u>Gaia</u>

- CI/CD: DevOpS methodology

  - <u>Pipelines</u>: Define and automate workflows

    - Child pipelines:

      - 1 per Spack environment
      - 1 per type of tests (App, Lib, prgEnv)   ~ 5 parallels jobs per pipelines

    - Multiple jobs in one stages

  - <u>Runners</u>: agents that execute CI jobs

    - Utilizing **20 concurrents runners**

    - Running on the `*/tmp*` **filesystem** of the **login node** (cross-compilation for AMD GPUs)
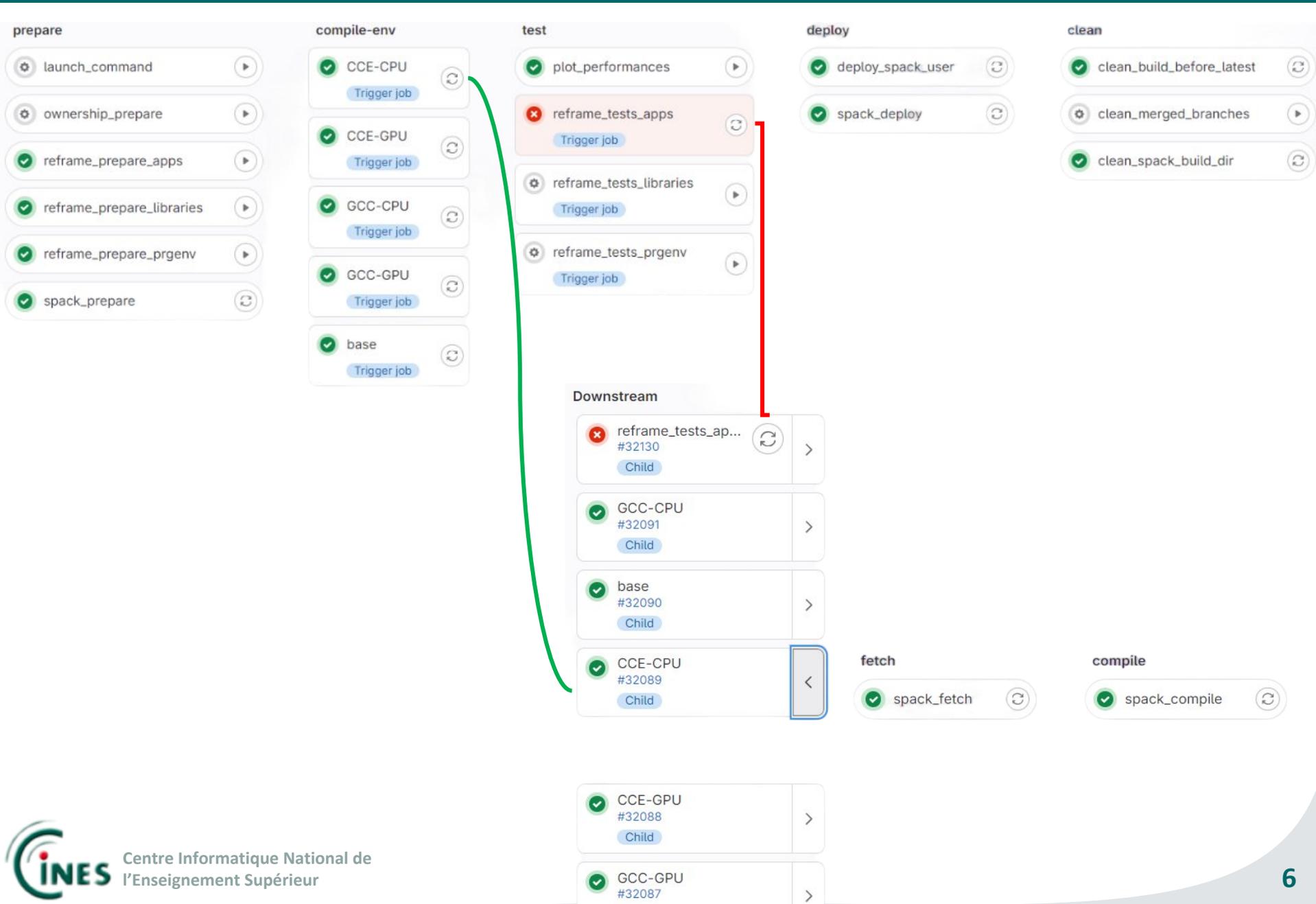
• **Spack**

- ▪ ***What is Spack ?***

"Spack is a package management tool designed to support multiple versions and configurations of software on a wide variety of platforms and environments"

- ▪ ***What is a Spack package ?***

*"Spack packages are installation scripts, which are essentially **recipes** for building (and testing) software."*

- ✓ *Where to find and how to retrieve the software*
- ✓ *Its dependencies*
- ✓ *Options for building from source*
- ✓ *Build commands.*

- ▪ ***Spack package list ?***
  - ▪ More than 7000 packages and recipes available : [list]

• **Spack in GAIA**

- ## *How ?*
  - ### **Git submodule** (*git clone --recursive*)
    - .gitmodules based on a version commit (updated every stable release)
  - ### **Internal recipe** (**local-repo**)
    - repos.yaml : Specifies repositories for prefered `packages.py`
  - ### **Modules:** Generated by Spack with an internal overlay to simplify the view of the modules
  - ### **Spack-user:** We provide users with a module `spack-user` with our configuration (no need for small installations).
- ## *Why?*
  - ### Benefit from contributions of other HPC centers (LLNL, Pawsey, KTH, etc.)
  - ### Promote CINES Through Spack Contributions:
    - #### Enhance the visibility of CINES by sharing recipes (`package.py`) with the Spack community. (~ 15 PR (thks to Etienne, Mohand, Mathieu and more to comes**)**

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- ## Spack in GAIA : Module view

```
---------------------------- /opt/software/gaia/prod/latest/Core ----------------------------
   CCE-CPU-3.1.0    GCC-CPU-3.1.0    develop           (L)     spack-MI250-3.1.0
   CCE-GPU-3.1.0    GCC-GPU-3.1.0    spack-GENOA-3.1.0

-------------------------------- /opt/software/gaia/deprecated ------------------------------
   CCE-CPU-3.0.0    CCE-GPU-3.0.0    GCC-CPU-3.0.0    GCC-GPU-3.0.0    archive (L)    user-CPU-3.0.0    user-GPU-3.0.0

---------------------------- /opt/software/gaia/prod/latest/Base ----------------------------
   anaconda3/2023.09-0    ffmpeg/6.0              hpcviewer/2023.07    metis/5.1.0-int64          papi/6.0.0.1
   benchmark/1.8.3        gdb/13.1               julia/1.10.0         metis/5.1.0         (D)    poppler/21.09.0
   blitz/1.0.2            gnuplot/5.4.3          libxml2/2.10.3       mmg/5.7.1                  qt/5.15.11
   bzip2/1.0.8            gsl/2.7.1              libxsmm/1.17         mpifileutils/0.11.1-mpi    zlib/1.3
   cmake/3.27.7           hpctoolkit/2023.08.1-mpi  likwid/5.2.2      nsimd/3.0.1

---------------------------- /opt/software/gaia/dev/latest/Core ----------------------------
   CCE-CPU-4.0.0    CCE-GPU-4.0.0    GCC-CPU-4.0.0 (L)    GCC-GPU-4.0.0    spack-user-4.0.0

---------------------------- /opt/software/gaia/dev/latest/Base ----------------------------
   gdb/14.1       (D)    hpcviewer/2024.02 (D)    paraview/5.13.0      r/4.3.0        sox/14.4.2
   gnuplot/6.0.0 (D)    papi/7.1.0              poppler/23.04.0 (D)    rust/1.78.0

-------------------- /opt/software/gaia/dev/3.1.0-05ab50b1/GCC-CPU-4.0.0 --------------------
   adios2/2.10.0-mpi    mumps/5.6.2-int64-omp-mpi    petsc/3.21.1-omp-mpi       siesta/5.0.1-elpa-omp-mpi       (D)
   boost/1.85.0-mpi     octopus/14.1-elpa-mpi        plumed/2.9.0-mpi           slepc/3.21.0-mpi
   cdo/2.4.2-omp-mpi    openblas/0.3.26-omp          quantum-espresso/6.8-omp-mpi  sundials/7.0.0-mpi
   hypre/2.31.0-mpi     openfoam/2312-int64-mpi      siesta/4.1.5-elpa-omp-mpi   superlu-dist/8.2.1-int64-omp-mpi

-------------------------- /opt/software/gaia/deprecated/.archive --------------------------
   CCE-CPU-2.0.0               CPE-22.11-rocmcc-5.2.3-softs    CPE-23.02-rocmcc-5.3.0-GPU-softs    user-CPU-2.1.0
   CCE-CPU-2.1.0               CPE-23.02-aocc-3.2.0-CPU-softs    GCC-CPU-2.0.0                      user-GPU-2.0.0
   CCE-GPU-2.0.0               CPE-23.02-cce-15.0.1-CPU-softs    GCC-CPU-2.1.0                      user-GPU-2.1.0
   CCE-GPU-2.1.0               CPE-23.02-cce-15.0.1-GPU-softs    GCC-GPU-2.0.0
   CPE-22.11-cce-15.0.0-softs    CPE-23.02-gcc-12.2.0-CPU-softs    GCC-GPU-2.1.0
   CPE-22.11-gcc-11.2.0-softs    CPE-23.02-gcc-12.2.0-GPU-softs    user-CPU-2.0.0
```

• **Configuration**

- ▪ **Use of spack environments :**
  - • Allows users to work within isolated groups of independent packages.
  - • Objective: To offer virtual environments (similar to Python venv) that enable users to share common installations.
  - • Designed for easy sharing and reuse by others and across different systems.

- ▪ **Configurations files :**
  - • compilers.yaml
  - • packages.yaml

  Most of the work has to be done here. It contains the default preferences for compilers and for providers of virtual packages, highly dependent on the system being used."

  - • concretizer.yam
  - • config.yaml
  - • modules.yaml

  Global configuration, with minimal dependence on the system.

  - • repos.yaml
  - • mirrors.yaml

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- **Interesting Spack features**

  - **Currently in use:**

    - **Upstreams**: allows you to point your Spack installation to another installation in order to use all the packages installed there

    - **Parallel builds:**

      - *« child pipeline » (spack ci generate)*

      - *Package level (make –j)*

    - **Spack binaries** (pre-built binary caches ~binary packaging: .rpm, .deb)

      - Installation times are reduced by around **20 times**!!

  - **To test again:**

    - *Spack containerize: «creates recipes to build images for different container runtimes»*

    - *Spack test: «run spack's tests for an install»*
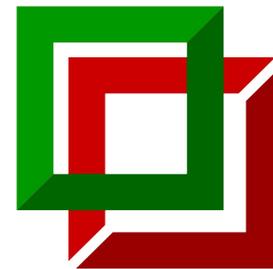
• **Reframe**

▪ *What is Reframe?*

"ReFrame is a powerful framework for writing system regression tests and benchmarks, specifically for HPC systems. Written in python"

▪ *How and where?*

- **Physically installed**, but intended to be used as a sub-module [coming soon]
- **Configuration**: setting.py files: describes the systems used (partition, the scheduler, etc.) and the "environments" (application environment to be tested)
- Internal **git** repository: cines-checks

▪ *For what purpose?*

- **Apps/Libs:** Monitoring and testing software installations deployed by spack
- **Prgenv:** verification of the programming environment deployed by HPE
- ~~**System** (IO, Slurm)~~
- ~~**Microbenchmarks** (HPL, OSU, HPCG, gpu_burn, ...)~~

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CP2K GPU Performance Over Time
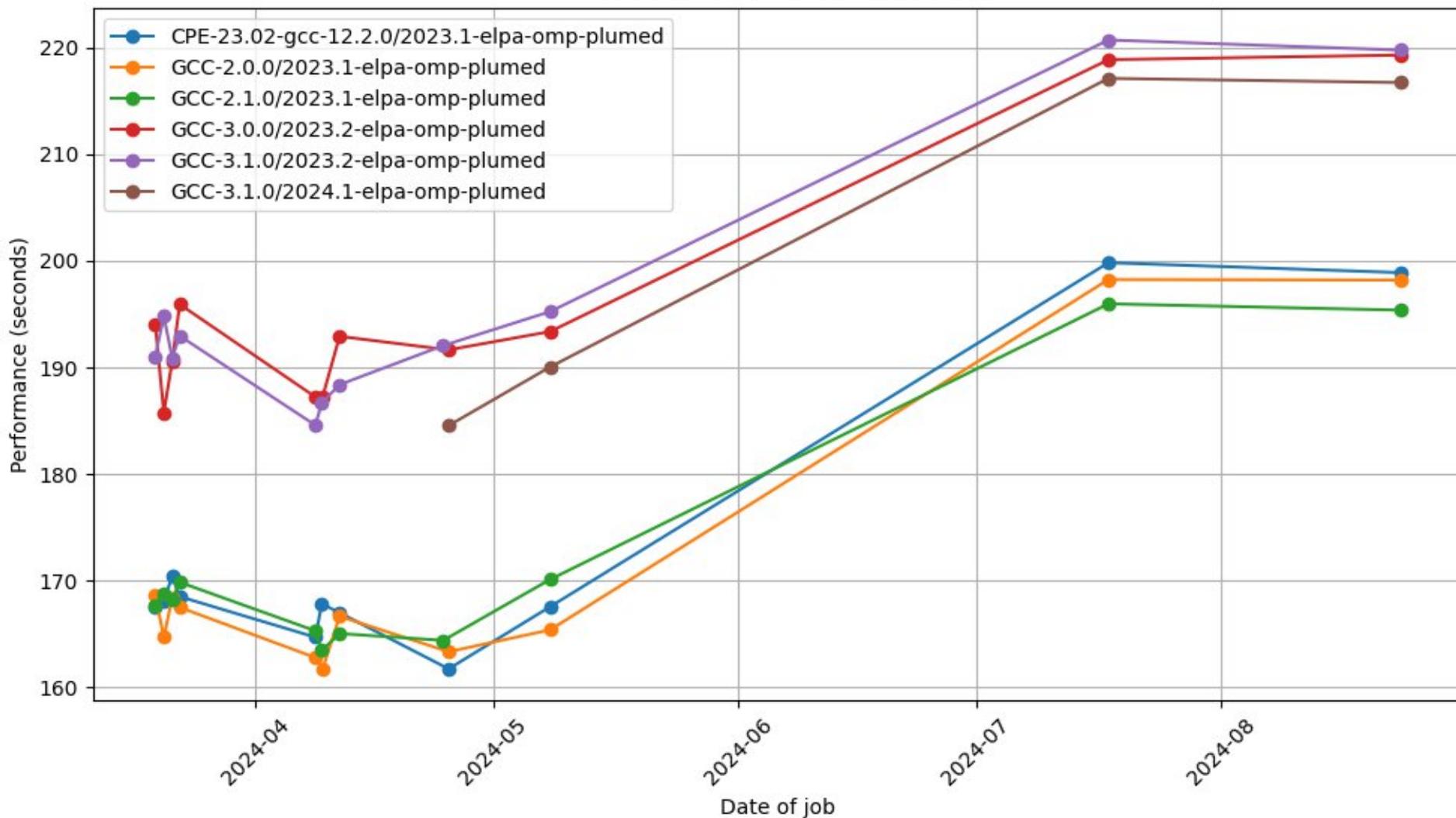
Thank you for your attention!

Questions?

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