interTwin WP5 & synergies with ESCAPE

Enrique Garcia
CERN Digital Twins Kick-off meeting
05 Dec 2022
interTwin WP5 tasks

- **Bi weekly** meetings, **Tuesdays at 10h00**

- **T5.1** Federated compute infra (HTC, HPC, Cloud, Quantum)
  - Provide **software solutions** to enable resource provisioning on the wide range of comp providers.
  - Lead by INFN (Diego Ciangottini)

- **T5.2** Federated data infra
  - Support **data requirements** of digital Twins.
  - Lead by DESY (Paul Millar)

- **T5.3** Federation services and policies
  - **Security and accountability** for users and providers
  - Lead by UKRI (Ian Neilson)

- **T5.4** AI-based orchestrator
  - **Orchestrate** data and compute **resources** "intelligently" (taking into account data location and performance metrics).
  - Lead by INFN (Marica Antonacci)
WP5 Heads up

- **Survey** (19 Questions) to providers (9 Nov) - start a button-up approach
  - Computing resources
  - Data and storage
  - Policies

- **Aim** is to receive input
  - Interfaces
  - Existing solutions
  - Ready to support R&D

- To date: 6 (out of 8) answers WP5 - Drive folder
  - PSNC, EODC, GRNET, IZUM-JSI, UKRI and FZJ

- F2F meeting at Madrid (Jan '23)
  - Align requirements, expected foreseen baseline, what needs to be extended...
T5.1 - Computing resources

- From survey:
  - In general all providers will contribute:
    - Cloud + HPC/HTC (batch system + Slurm - mainly) computing resources.
  - Most entering the Peta/Exascale, other “smaller”.
  - Some providers support CVMFS (framework to bring software to sites).
  - Most providers allow container execution (apptainer, Singularity, udocker).
    - With some limitations (see policies)
T5.1 - Computing resources

- From WP5:
  - Open discussion / brainstorming. Lots of points to be aware of:
  - HPC and HEP use-cases will be different!
    - **HPCs:**
      - High degree of communication between sites + nodes
      - Generally **optimised** for different HPC architectures.
      - Exposing details of HPCs architectures is what abstraction layer tends to do.
    - **HEP:**
      - High level of parallelisation (no cross-node communication)
    - **HTCondor** the solution for both?
    - We should be aware of bandwidth limitation between sites.
  - CVMFS and containers
    - **Potential overlap** (but limited by site policies - root privileges /internet connection)
      - **Combination** of both can be ideal.
    - Mounting different FS on HPC systems / workers nodes (problem to be investigated)
T5.2 - Data and storage infrastructure

- **From survey:**
  - Heterogeneity
    - Plenty of storages, configurations and file transfer protocols.
    - Some *caching architectures* implemented in certain sites.

- **From WP5:**
  - Ongoing discussion between WLCG (ESCAPE data lake) model and DEDL (DestinE Data Lake) infrastructure.
    - DEDL still *partly in design phase*. From first discussion:
      - Stronger knowledge architecture: expected Jan '23.
      - Procurement-driven. No large data movements planned - *co-locate computing resources close to storage*. How resources will be collocated?
    - ECMWF is responsible of the app that will run in the DEDL.
    - EUMETSAT provides de platform
  - Use cases should come from core (WP6) thematic modules (WP7)
T5.3 - Policies

- From survey:
  - Heterogeneity. No major commonalities either
  - No common/defined AAI framework
    - Common ground: HPC are happy to grant access to people using federated identities (EOSC Future AAI model ?)
  - Neither monitoring infrastructure.
  - Some providers do not allow root privileges
    - Others do not allow internet connection to computing nodes...
    - Connection through ssh and just following data center policies
T5.4 - AI-based orchestrator

- Not addressed yet
Synergies with ESCAPE

● **Data management.**
  ○ If chosen, the Data Lake infrastructure:
    ■ **RUCIO** instance (should interTwin use the same one?)
      ● FTS (File Transfer System)
      ● Gfal2
      ● CRIC...

● **Software.**
  ○ Everything points to the use of CVMFS in interTwin.
  ○ ESCAPE: No distributed/federated software instances.
    ■ Multiple container registries, git instances, heterogeneity in "good practices"/software lifecycles

● **Use of Analysis platforms / Running workflows and pipelines.**
  ○ Missing common ground. Dependent of the experiment / collaboration / field.
Synergies with ESCAPE

● Analysis platform.
  ○ ESCAPE provided a toolkit to be used in different partners resources.
  ○ CERN team:
    ■ Built an analysis platform.
    ■ Connected to the ESCAPE Data Lake (ESCAPE RUCIO instance, based on WLCG)
    ■ JupyterHub interface (notebook service)
      ● Hide DL complexity
      ● Allows interactive analysis and use batch systems
    ■ Connecting with computing resources
      ● local cluster
      ● remote resources (Cloud + HPC + [HTC])
    ■ Running end-to-end workflows (testing Reana)
      ● Workflow definition (need to satisfy everybody needs)
ESCAPE/EOSC Future VRE tech horizon

- Virtual Research Environment (VRE)
- Moving current infrastructure towards an IaC deployment (terraform).
- Connecting with (more) remote computing (EOSC) resources.