Porting the IRCCS Sant'Orsola Computational Genomic platform on INFN Cloud: a first proof of concept



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The **5 research lines** and the National Scientific Committee











Knowledge **Transfer**

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ENERGY AND SAAF

MONITORING GAS EMISSIONS MONITORING CONCENTRATIONS OF DUST IN AIR SOIL RADIOACTIVITY MAPPING **CLIMATE ANALYSIS**

MONITORING RADIOACTIVE WASTE VERY LOW RADIOACTIVITY MEASUREMENTS

> HADRON THERAPY AND BNCT TO TREAT CANCER **PET & NMR DIAGNOSTICS DEVELOPMENT OF NEW RADIOPHARMACEUTICALS** DOSIMETRY FOR DIAGNOSTICS AND THERAPY

> > THE OF CULTURAL HERITAR NON-DESTRUCTIVE ANALYSIS DATING HISTORICAL/ARCHAEOLOGICAL FINDS ANALYSIS OF AUTHENTICITY

MEDICINE





OGY AND CHEMISTR,

RADIOBIOLOGY

ADDITIVE MANUFACTURING

SPACE COMPONENTS ANALYSIS

SPACE SENSORS AND DEVICES

ISOTOPIC LABELING

FUNDAMENTA





Enhanced Prlvacy and Compliance (EPIC) Cloud

- The GDPR states that Clinical and medical data (for instance, genomic) is personal data. Thus, it fits in the Art.9 special categories of personal data.
 - Genomic data is mostly impossible to be anonymized → GDPR shall always be applied
 - ISO/IEC 27001 is the main certification mechanism compliant with GDPR requirements (Art. 43, 58, 63)
- To comply with the requirements of health research projects INFN is involved in, we created a portion of the INFN Data Cloud infrastructure, applied specific organizational and technical security measures, and certified it ISO/IEC 27001, 27017, 27018.
 - This is the EPIC Cloud: a reference Cloud implementation for the treatment of sensitive data at INFN.

From the Data Controller side, the fact that EPIC Cloud is ISO-certified is a way to demonstrate that processing is performed in accordance with the GDPR.

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INFN - IRCCS Sant'Orsola Collaboration

Joint research agreement with the following objectives

- secure applications for genomic data
- GPU based solutions for genomic analysis methods
- federated and integrated cloud platforms for omics data
- adaptation of genomic pipelines to cloud and data lake architectures based on microservices
- Integration of omics data and other clinical data like Electronic Medical Records (EMR)



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Benchmark workflow

- Workflow designed to detect germline variants on whole genome sequencing data
- File types: .bam, .fastq, .gvcf
- Software containerized using custom
 Docker image
 - Burrow-Wheeler Aligner
 - <u>Samtools</u>
 - Genome Analysis Toolkit
- ~100GB of input genome per sample
- ~100GB of output files per sample
 - BAM file (Binary Alignment Map format)
 - Quality metrics
 - GVCF file (Genomic Variant Call Format)
- ~ 0.5 TB of temp files

Current Computing Architecture

Architecture

- Monolithic Infrastructure based on big Virtual Machines
- Snakemake as workflow manager
- SLURM as batch system
- <u>Conda</u> as package and environment management system

Issues

- Low scalability
- Low availability
- Not "elastic"
- Security concerns

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Where we are going

- OpenStack laaS
- Microservices approach (containers)
- Kubernetes/RKE2 cluster
- Nextflow workflow manager
- Prometheus/Grafana
- CI/CD and private container registry
- Automation tools (Puppet, Ansible, etc...)

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Kubernetes – RKE2

- Distributed Environment
- High Availability and Resilience
- Elasticity
- Wide community
- Well and continuously maintained
- Focused on security
- Hardening presets
- CVEs and interventions regularly published

The Cluster

- 3 Master Nodes 4 CPU, 8GB RAM
- 3 Worker Nodes 8 CPU, 16GB RAM
- 1 Worker Node 40CPU, 80GB RAM
- 3 Persistent Volume Claims (1 TB each)
- 1 Bastion 8 CPU, 16GB RAM

Nextflow + K8s

X nextflow

- General purposes Workflow Manager
- Well supported and widely adopted by the bioinformatics community
- Native support of containers
- Native support of Kubernetes (also Snakemake)
- Native support of K8s Persistent Volume Claims (PVC)
- Node selectors (CPU, GPU, "small", "medium", "large" nodes etc)

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Nextflow vs. Snakemake

X nextflow

- Pipelines written in Groovy
- Full support of containers
- The exact same workflow can run both locally or on the cloud
- Native support of Kubernetes with high customization
- K8s images cache friendly
- Native support of K8s Persistent Volume Claims (PVC)
- Data produced by previous steps is already visible to the next pods without additional transfers

- Pipelines written in Python
- Heavily focused on Conda environments
- Container support limited to docker-indocker
- Images cannot be cashed by K8s
- Persistent Volume Claims not supported
- Storage I/O tight to S3/SFTP transfers
- Each pod must download/upload hundreds of GBs of data per each step

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POLICI INICO DI **Sant'orsola**

Nextflow vs. Snakemake

X nextflow

- PVC configured as NFS volumes mounted on worker nodes
- PVC mounted directly to the pods
- Pods spawned as "native" docker images

- Files downloaded/uploaded to S3-like storage
- All pods spawned as Snakemake Docker image
- Software is run as docker-in-docker on top of it

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Monitoring (Prometheus & Grafana)

- Deep insights of the workflows
- Enables accurate debugging of the single steps
- Enables the optimization of resource utilization by each step
- Discovery of bottlenecks
- Comparable and consistent benchmarks and results

Monitoring (Prometheus & Grafana)

Conclusions

- The migration from a "classical" monolithic architecture to a more flexible, even though more complex, cloud architecture reveled to be promising
- Initial overhead to build the infrastructure
- Complex infrastructure but it offers high availability, scalability and elasticity
- The adopted "microservices" paradigm offers portability since the same workflow can be run on from a small laptop up to full-size computing cluster
- User friendly for the operator/researcher who submits the jobs
- Full-fledged monitoring platform to enable deep insights about job runs, performance and optimizations
- Better security due to a better control of the employed software and Vulnerability Scans of the Docker images

Future Outlooks

- Integration of and Identity Provider (IdP) tool such as Keycloak, FreeIPA or INDIGO IAM
- Integration of Galaxy as user friendly frontend to launch jobs
- Integration with object storage solutions to store the output files
- Stress tests
- Exploration of queue managers
- Mirroring of architecture to the Baseline tenant

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