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PROviding Computing solutions for ExaScale ChallengeS

Towards a New Paradigm for Programming Scientific Workflows

Reginald Cushing, Onno Valkering, Adam Belloum, Cees de Laat

24th Sep 2019, eScience conference – BD2DC, San Diego



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 777533.



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PROCESS LOFAR: Low Frequency Array



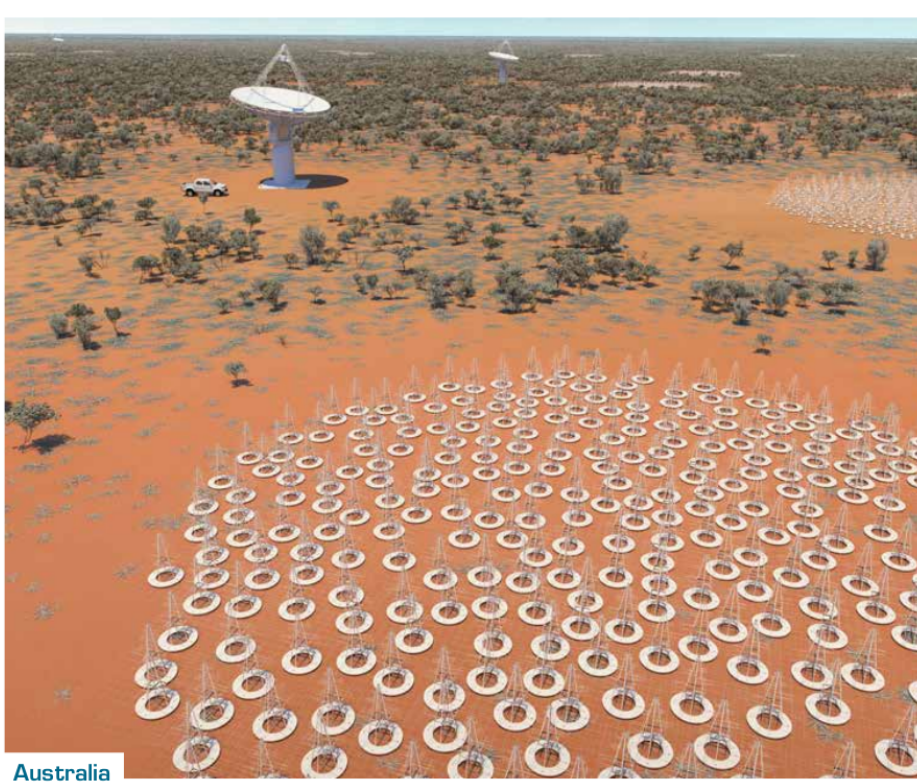
Images courtesy of: ASTRON

LOFAR radio telescope – is a “distributed software telescope” consisting of ~88.000 antennas in ~51 stations scattered over Europe. It produces up to **1.6 TB/s of raw data**, processed real time to combine the signals of multiple antennas (correlation). **This results in up to 35 TB/h of intermediate data** (visibilities) which is stored for further analysis.

PROCESS SKA: Square Kilometer Array

On an unprecedented scientific scale across two continents, the SKA will revolutionise our understanding of the Universe.

South Africa



Australia

Operational in 2022+

130K ~ 1M (LOFAR-style) antenna in Australia + 200 ~ 2000 dishes in South Africa

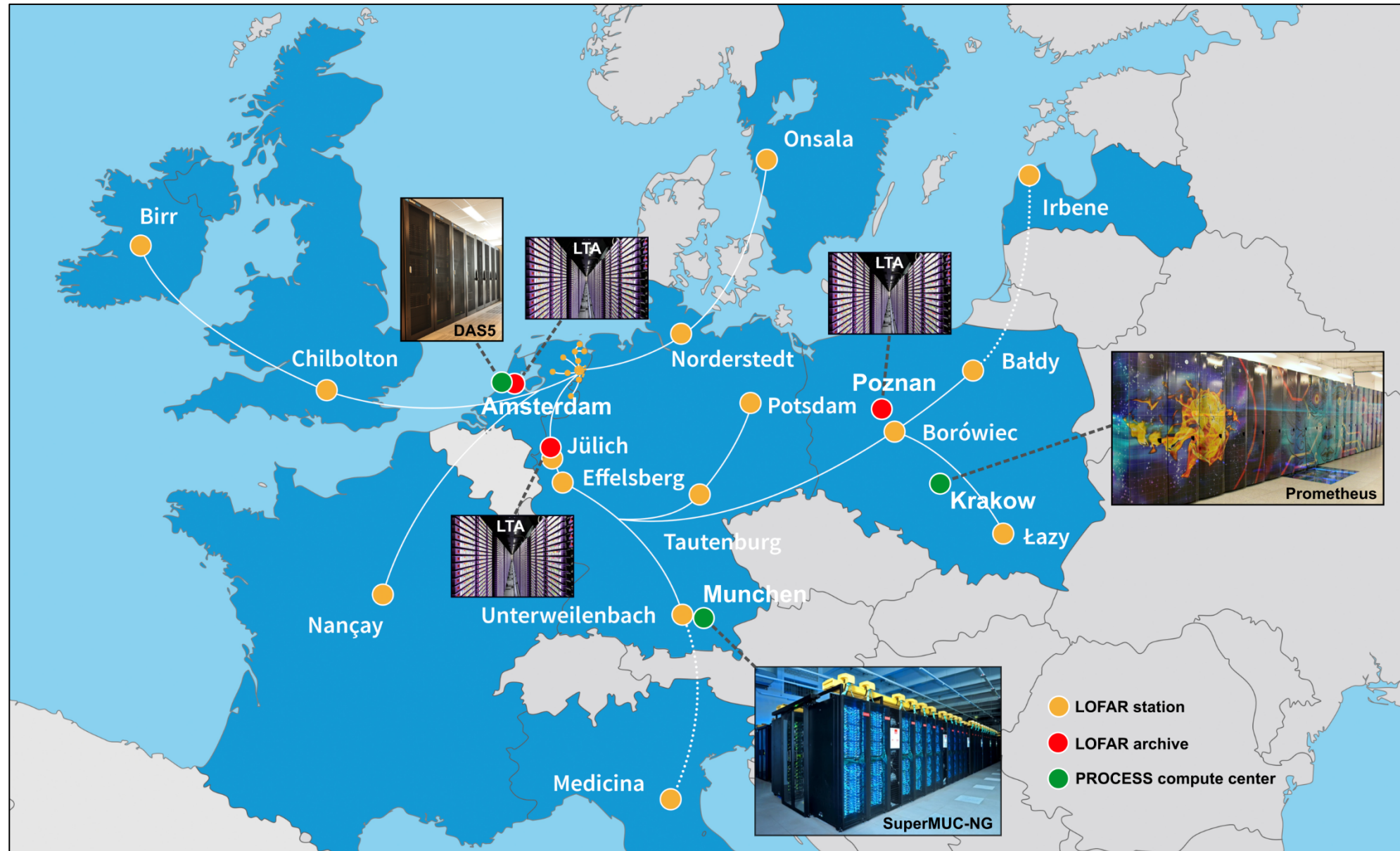
Wider frequency range and higher sensitivity and survey speed than existing telescopes

Zettabytes/year **raw** data volumes

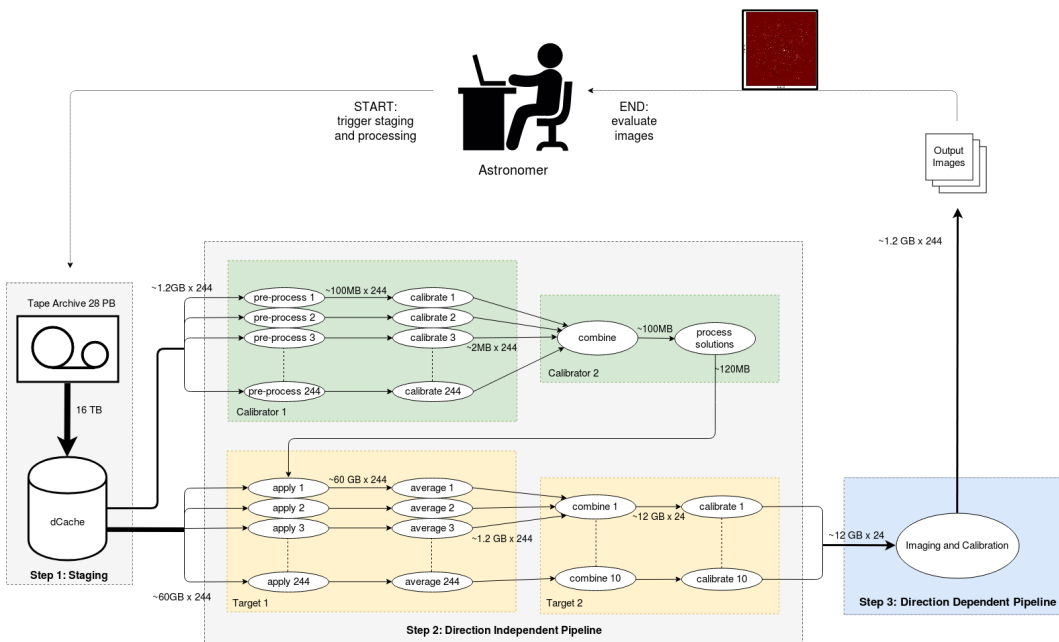
130~300PB/year of correlated data

Huge data and processing problem

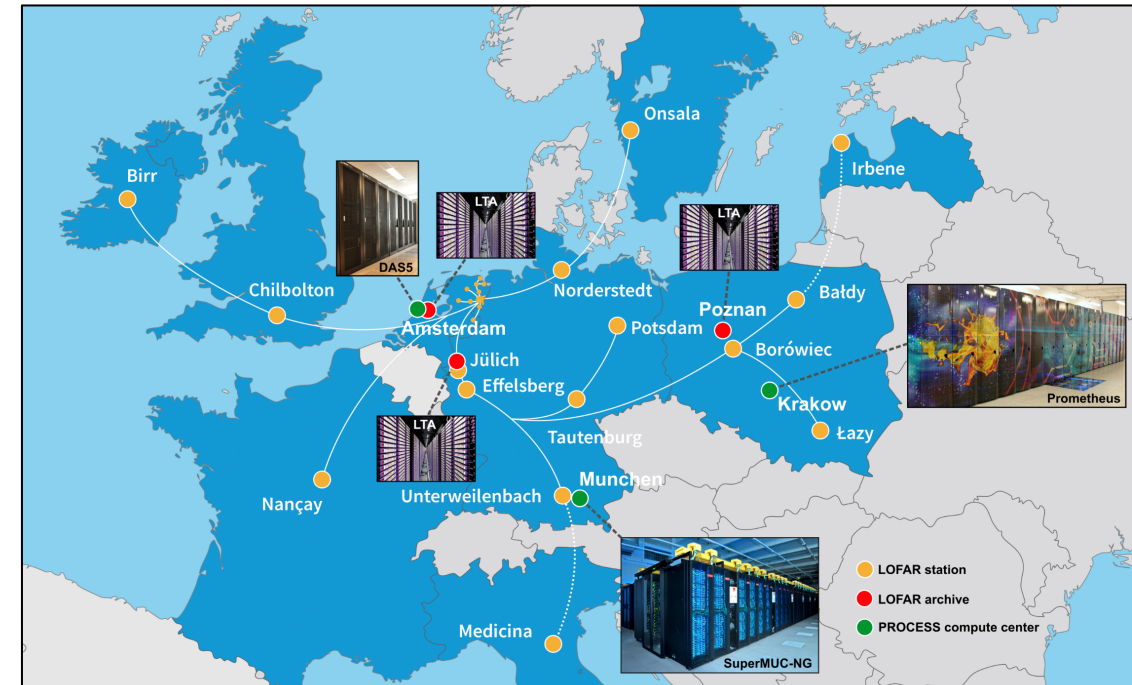
PROCESS Overview of hardware locations



Applications



Dispersed Resources



Complex Mapping

- **Application**

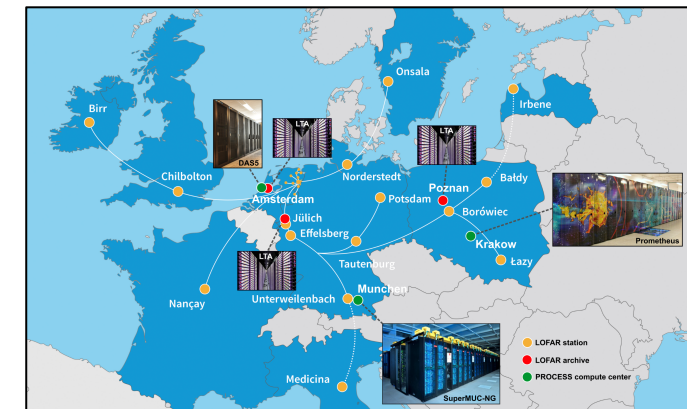
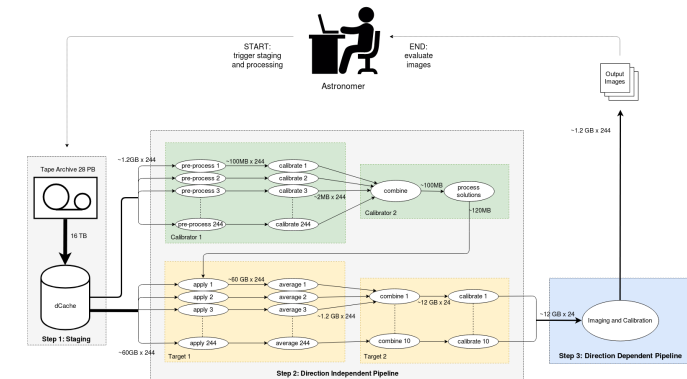
- How to facilitate rapid pipeline development and deployment on heterogenous resources?

- **Infrastructure**

- How to setup complex infrastructures that can facilitate applications in their requirements?

- **Middleware**

- How to scale applications from locally tuned clusters to multi-datacenter deployments?

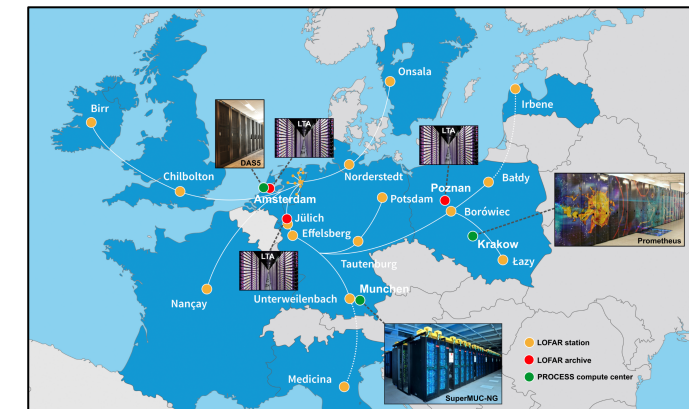
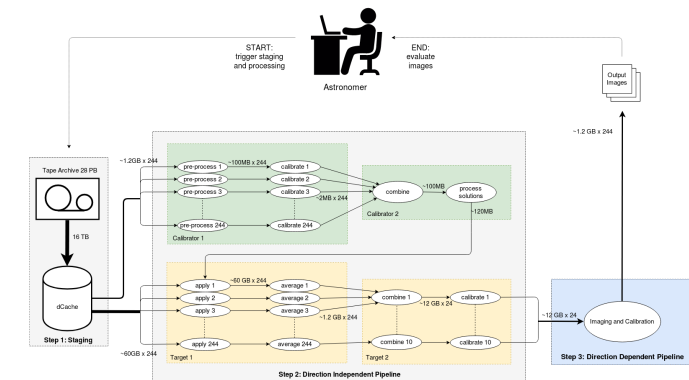


- **Data**

- How to smartly transfer data to make the most of the underlying infrastructure.

- **Security & Privacy**

- How to create secure scientific pipelines that process sensitive data on distributed infrastructures using dispersed resources?



- **Challenges cover all layers**

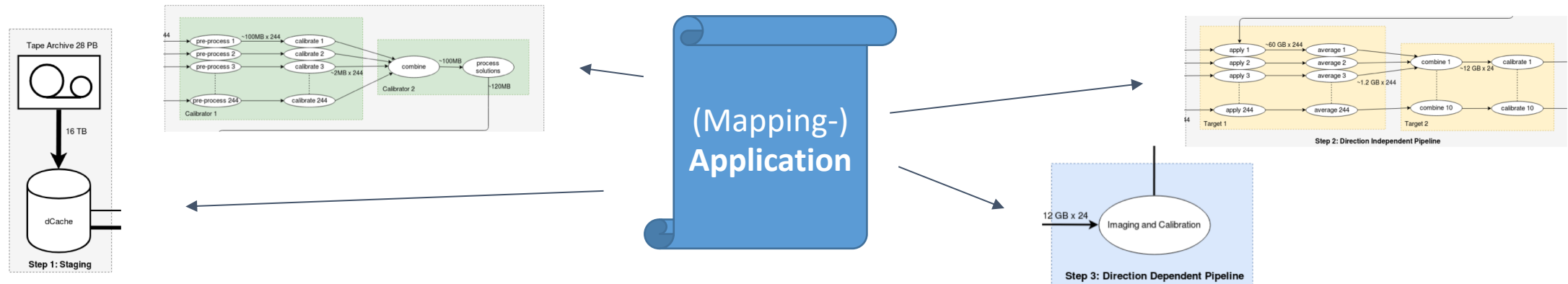
- In order to address these challenges it is required to control the entire stack, i.e. both applications and networking.
- A full-stack approach lets us fine-tune the interaction between application and dispersed resources.

- **Workflow Management Systems ?**

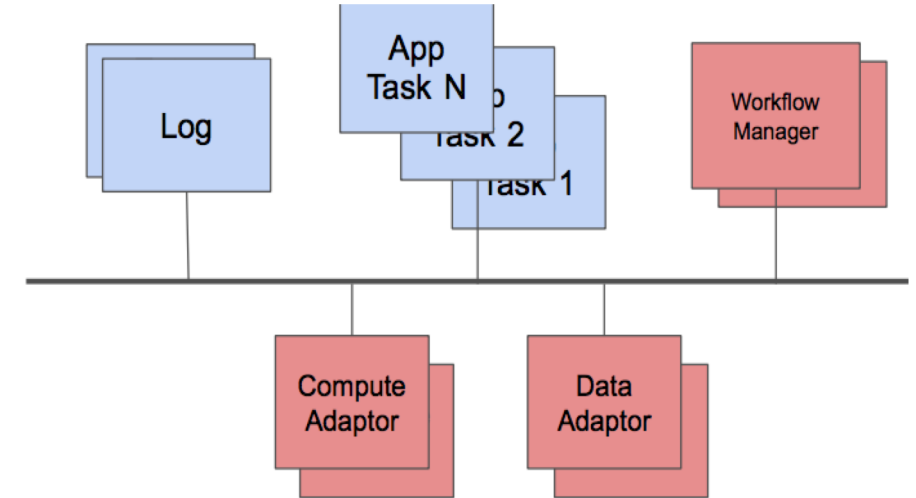
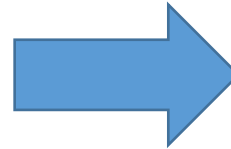
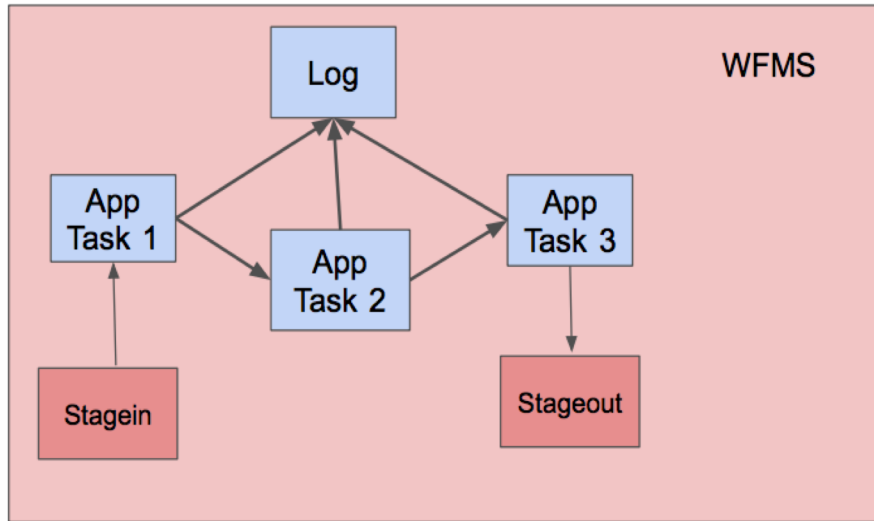
- Traditional workflow systems don't model the underlying infrastructure, and usually target a static deployment.
- We need a more expressive language than typical flow-charts.

• Programmability

- Higher-level programming languages and DSLs are known to be very expressive, while still being relatively user-friendly.
- These can be used to describe the complex mapping between applications and resources. Essentially making the turning the (mapping-)application into the orchestrator:

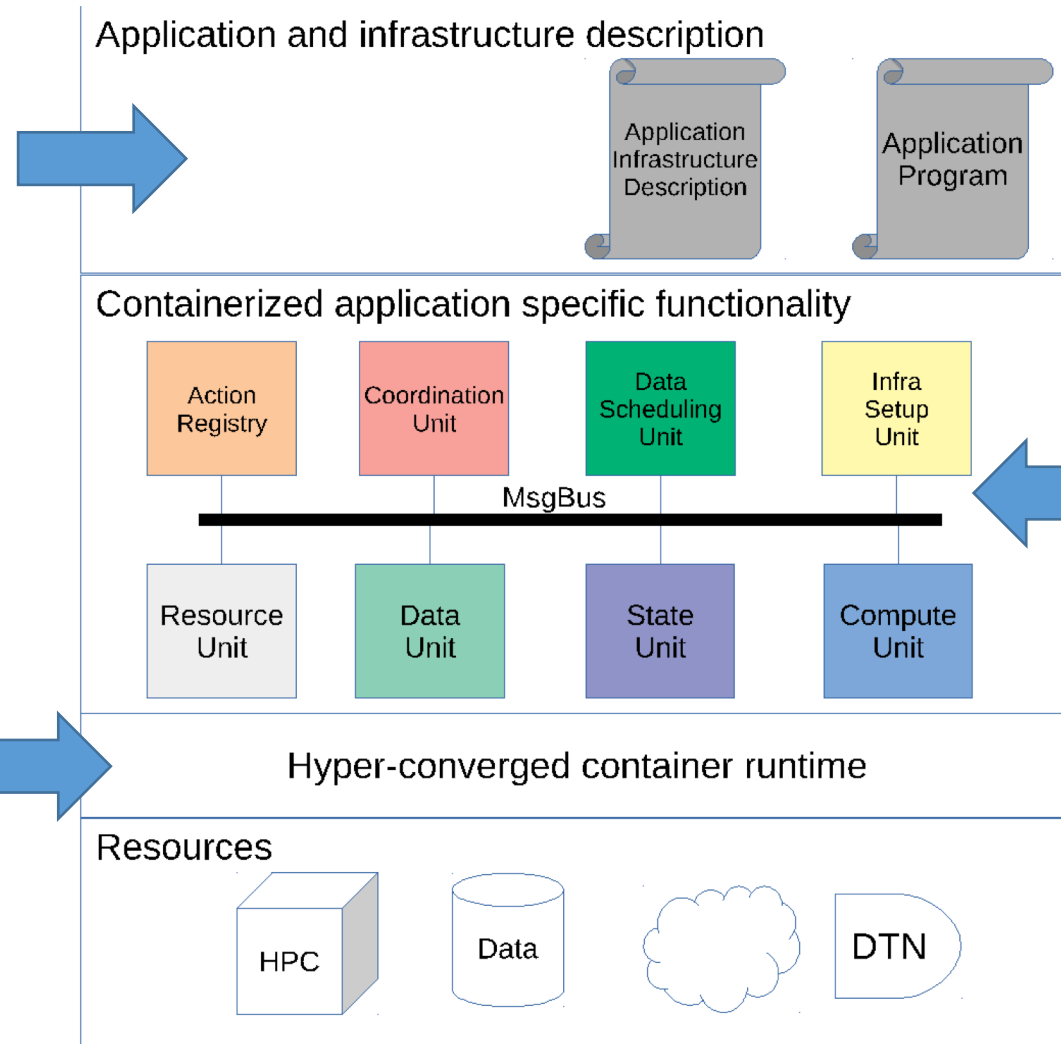


- Move towards a flat and container-centric micro-architecture.



- **Adaptable** through a hyper-converged container runtime.
- **Dynamic** through programmable application orchestration.
- **Efficient** through on-demand provisioning and elastic scaling.

Applications are leading for what components will be provisioned.

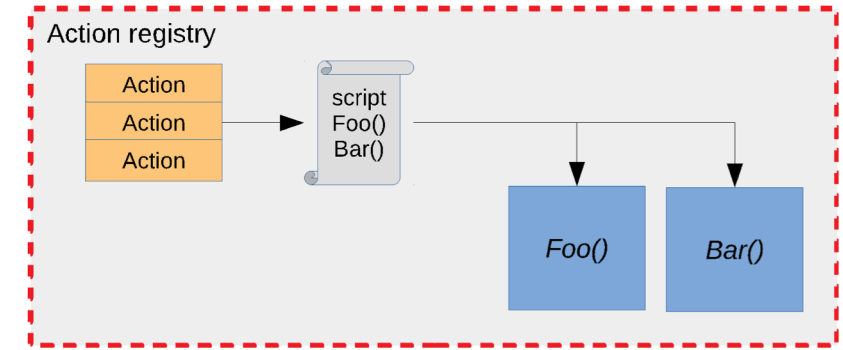


Choreography is effectuated though an reactive and event-driven (mapping) application.

Container runtime abstracts away from heterogeneous and dispersed resources.

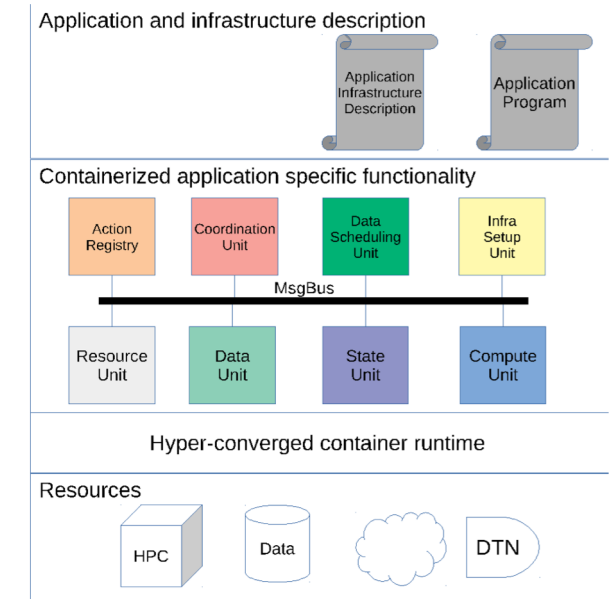
- **Containerized functions**

- Encapsulates arbitrary compute routines
- Docker for Cloud, Singularity for HPCs
- Specify the functions that are exposed by the services or compute routine.



- **Registry of functions**

- Keeps track of the available functions
- Used for discovery and documentation
- Composable building blocks



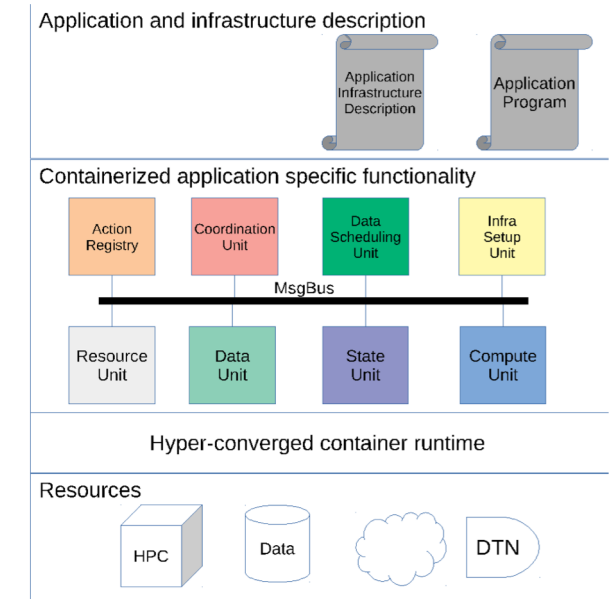
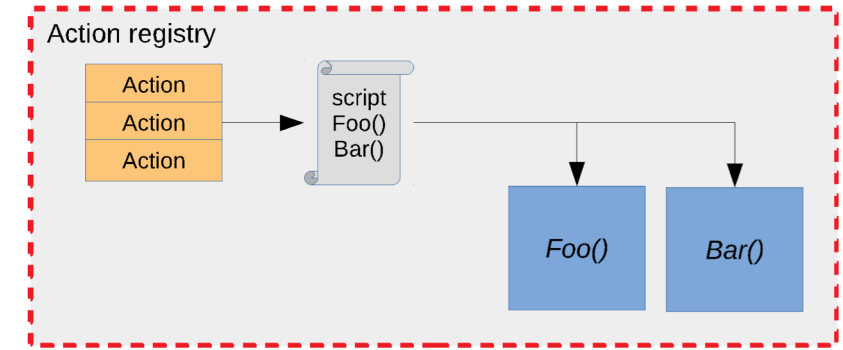
- **Coordination scripts**

- Hierarchical compute routines
- Using an existing/familiar language
- Registered in the registry

- **Import containerized functions**

- Generated stubs are used to represent containerized functions inside the IDE.

```
import { stage } from './lofar-lta';  
  
stage[2432018]  
stage(observation: number): string[]  
The ID of the observation  
This function stages an observation at the LOFAR LTA.  
@return — An array of SURLS of the staged files.
```

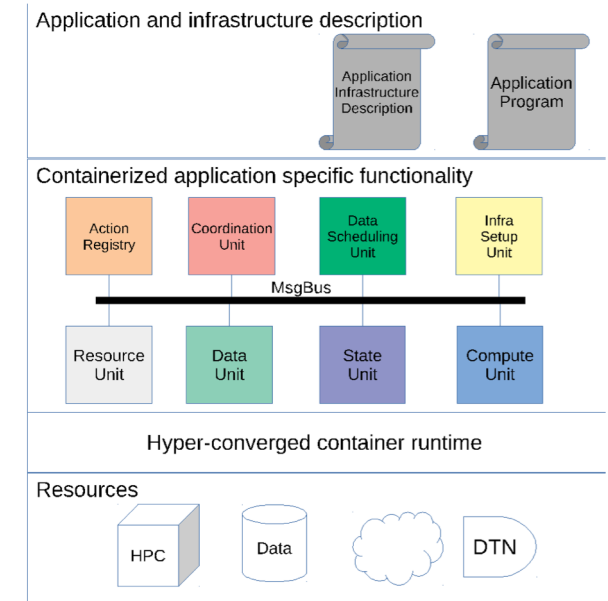
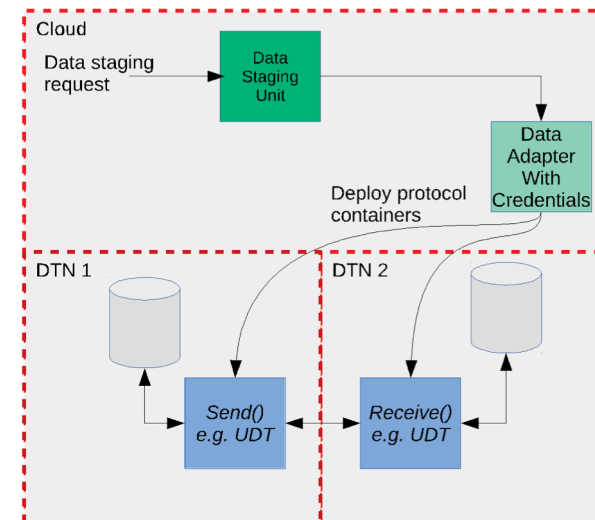


- **Coordinator / Infrastructure Units**

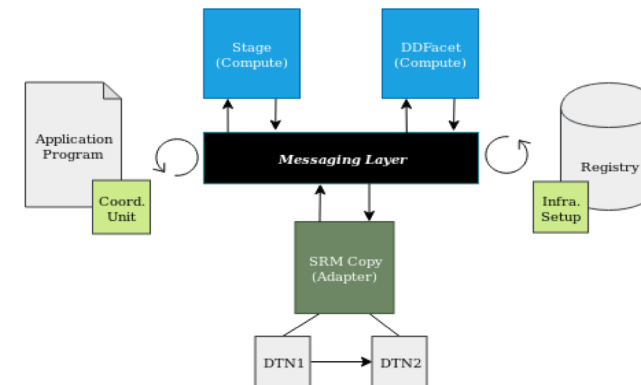
- Starts the application by generating initial events.
- Contributes the event-loop to process events.
- Resolves events to function-execution invocations.

- **Data Unit**

- Resource access is abstracted through adapters containers.
- Transfer between dispersed locations using DTNs.



- Challenges of future scientific applications stem from all layers of the stack. Programmable micro-infrastructures allow us to address all of these challenges.
- Outlined the basic components that are needed to create isolated, portable and scalable micro-infrastructures.
- **Future work**
 - Implementing a proof of concept based on the reference architecture.
 - Open-source and available on GH: <https://github.com/brane-ri>



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