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Architectures and Tools for Large-Scale Workflows Exa-AToW

November 27, 2024

<https://numpex.org/>

<https://exatow.fenix.rudi-univ-rennes1.fr/>

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Partners & Roles

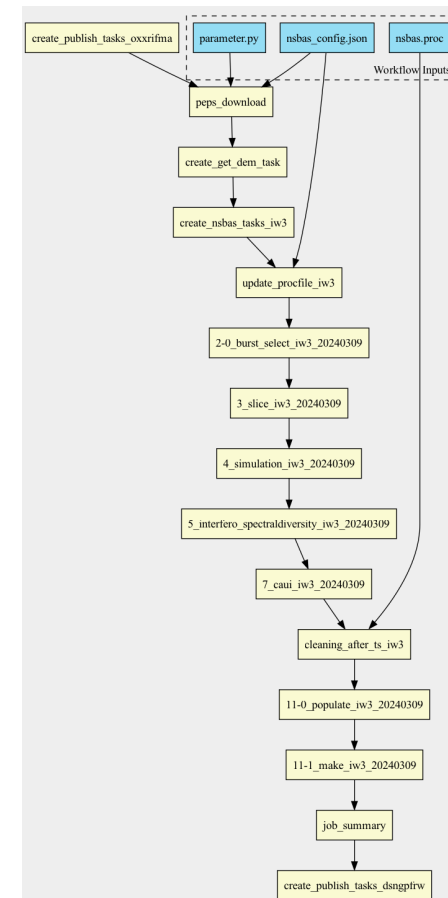
- University of Rennes
 - PI: François Bodin / Mark Asch
 - Role: Architecture
- Inria DataMove
 - PI: Olivier Richard
 - Role: Orchestration
- CEA DRF
 - PI: Thierry Deutch
 - Role: Workflow specification
- CNRS IDRIS
 - PI: Guillaume Harry
 - Role: Cybersecurity
- CNRS PYTHEAS
 - PI: Didier Mallarino
 - Role: Sustainability models

Co-coordination:

- François Bodin
- Thierry Deutsch
- Mark Asch



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Src: NSBAS

Estimation des déformations du sol
par imagerie satellitaire radar

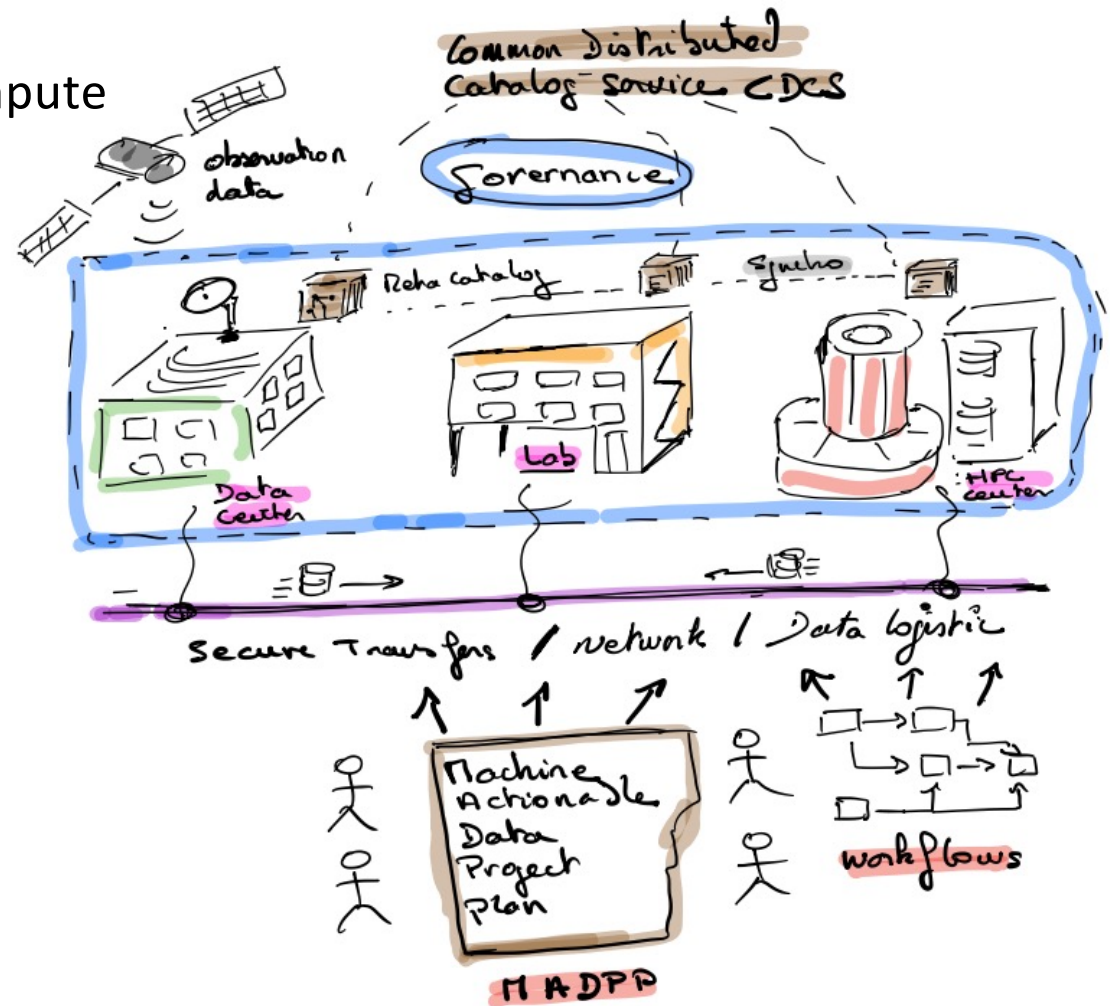
Project Components Overview



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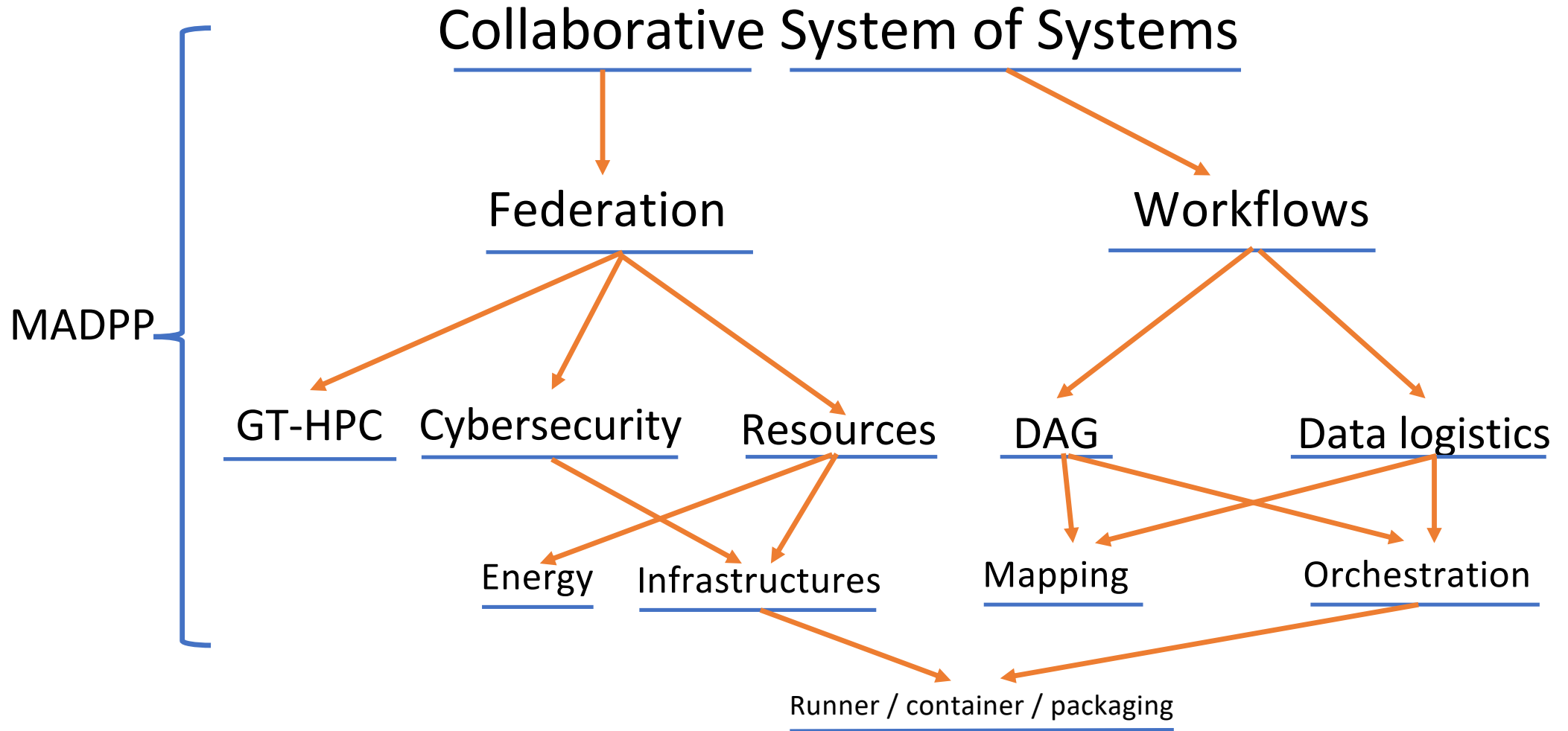
1. Federation of network, data, and compute resources
2. Metadata Centric Approach
3. Machine Actionable Data Project Plan (MADPP)
4. Data Logistic
5. Application & Workflow Support
6. Federation Governance



Exa-AToW in a Nutshell



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The Exa-AToW Challenges

- **D1** How to dynamically allocate distributed resources to accommodate for variations in the power cost
- **D2** How to organize data logistics, data life cycle, data processing, and metadata *standardization*
- **D3** How to ensure cyber-security at a large-scale on heterogeneous technologies
- **D4** How to deal with the hardware and software heterogeneity in order to run in a repeatable, replicable, and reproducible manner (and thus improving reusability)



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Current status

Collaborations linked to use-cases

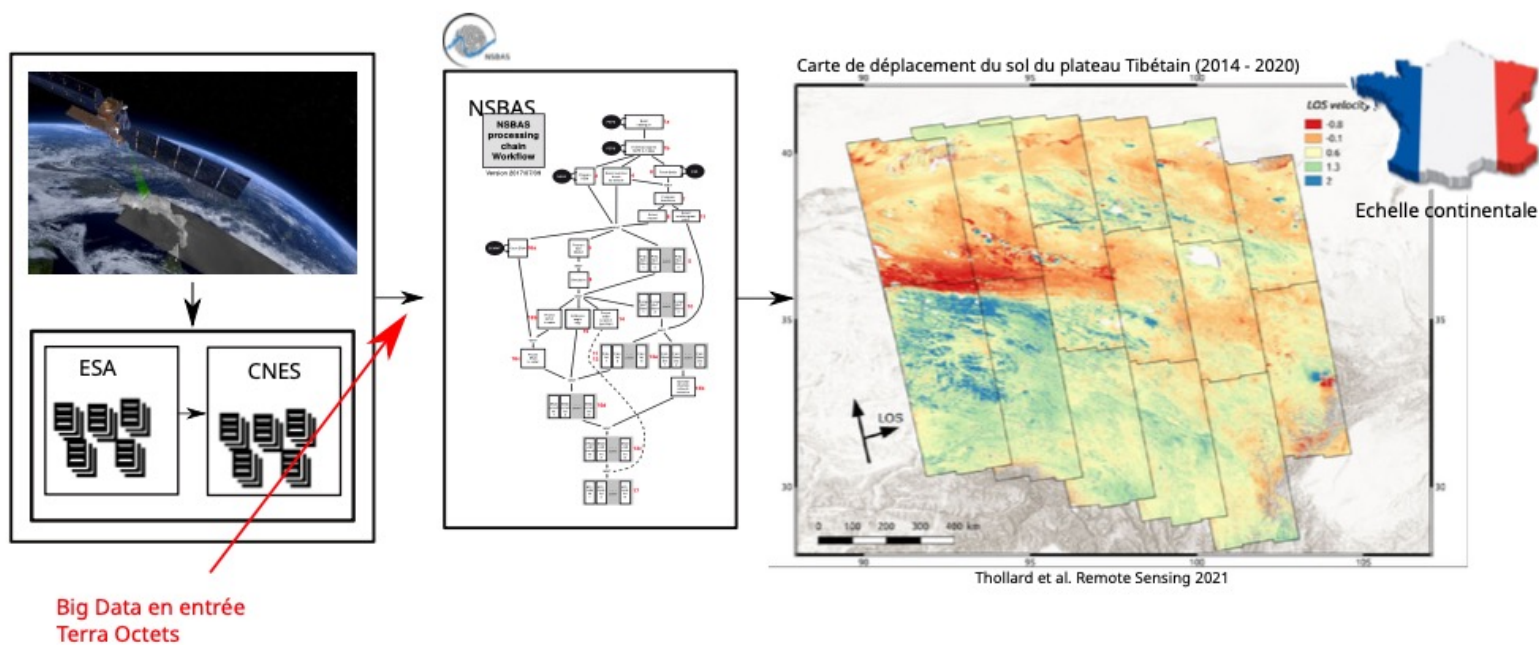


- SKA
 - Eclat (<https://eclat.cnrs.fr/>)
 - “centre d'excellence sur le calcul haute performance et l'intelligence artificielle au service de l'instrumentation pour l'astronomie”
- Data Terra / Gaia Data
 - NSBAS use-case (<https://www.mdpi.com/2072-4292/13/18/3734>)
 - Processing Chain Used in the FLATSIM Service
 - Machine Actionable Data Project Plan
- PEPR Diadem
 - Material simulation (<https://www.pepr-diadem.fr/> project Diamond)

Imagerie radar

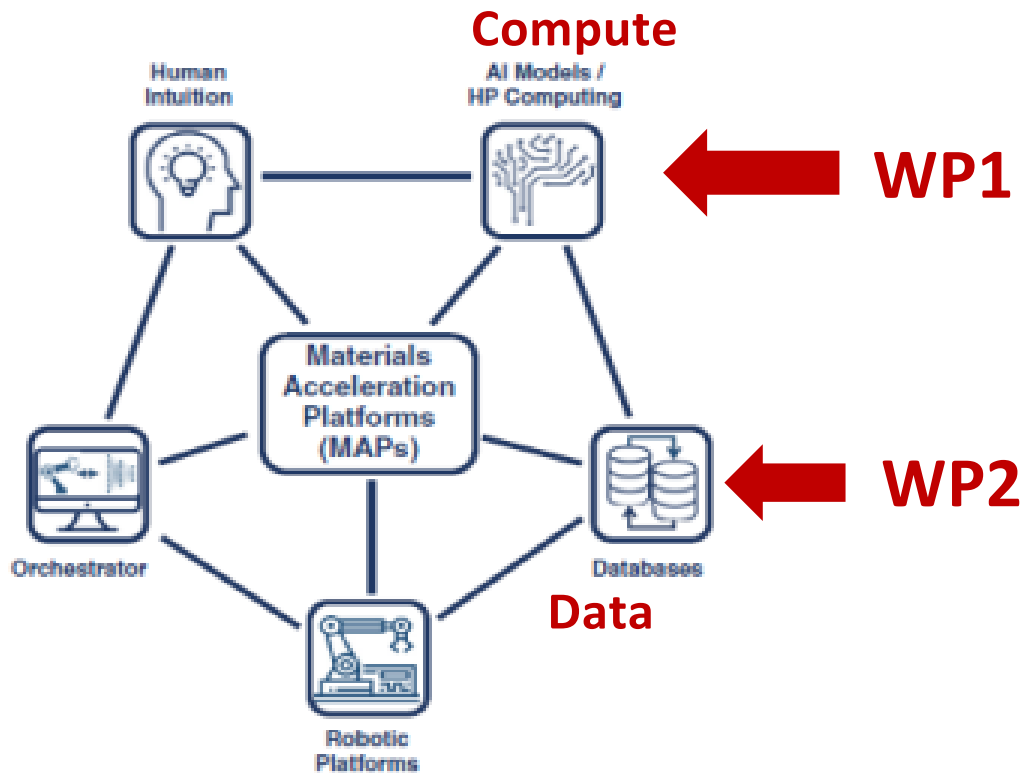
Les problématiques

NSBAS





TARGETED PROJECT DIAMOND OF THE DIADEM PEPR



- Infrastructure Project
- HPC Aspects (GPU porting, workflow) addressed in the NUMPEX PEPR
- DIAMOND does not provide computing resources (see GENCI)

Role of Artificial Intelligence (AI):

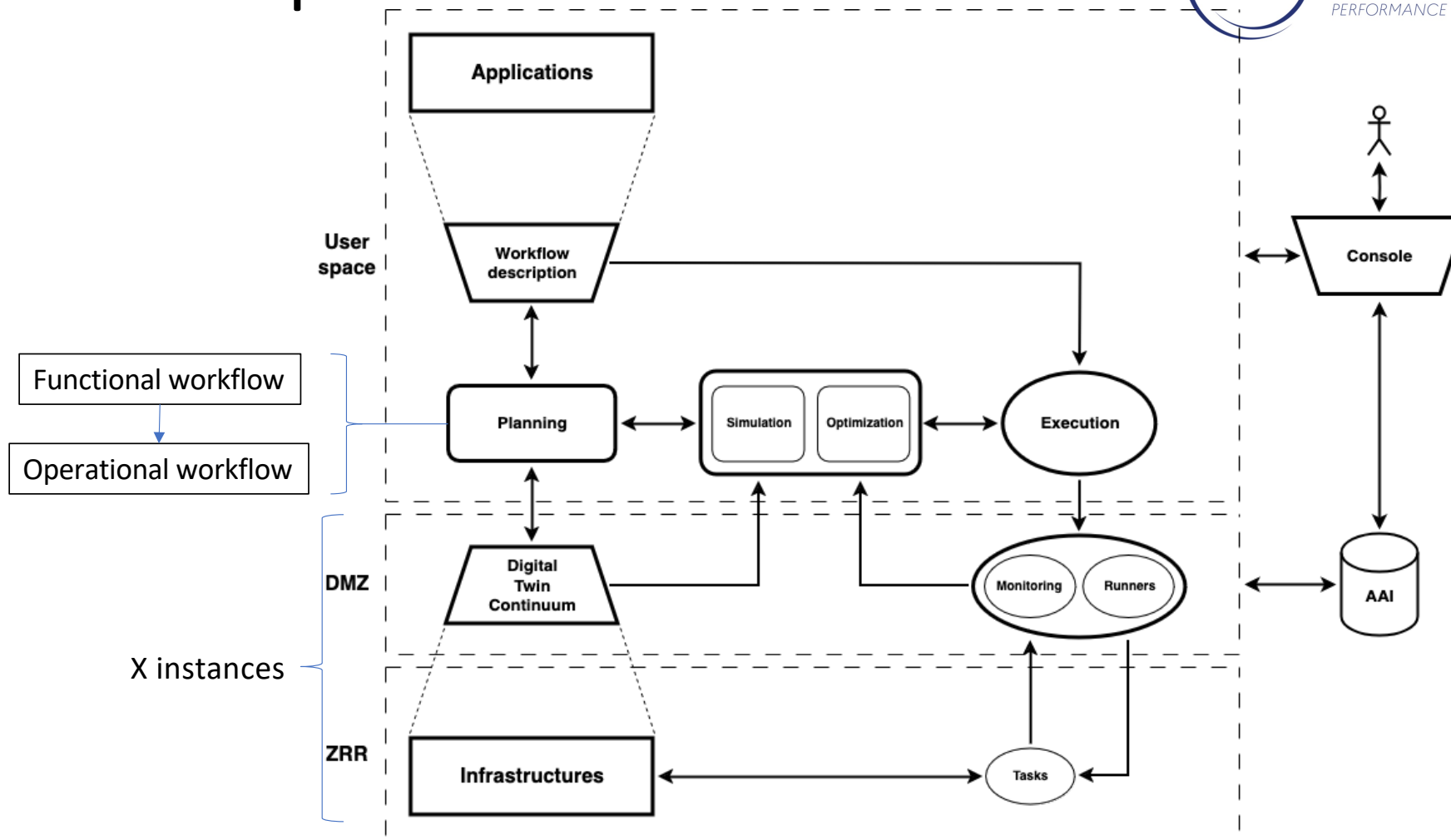
- Enhancement/acceleration of simulation (WP1)
- Integration into material workflows (WP1)
- AI toolbox for data analysis (WP2)

Next Steps Focus



- Machine Actionable Data Project Plan (MADPP)
 - Specification workshop 21-22-23 of August Exa-AToW / Data Terra
- Experimental platform
 - AAI (Keycloak deployment)
 - Federating resources: Eskemm nodes, TGCC Cluster nodes, Turpan nodes, Slices nodes, ...
 - Multi-agent based simulations
- AI integration
 - Dynamic workflow management and resources allocation
 - Exa-AToW RAG (LLM) database deployment
- **DDF Pipeline @TGCC experiment**
 - **Data logistic and computation experimentation**
- NSBAS @CNES-Idris experiment
 - Large scale NSBAS computation
 - Data logistic experimentation

Next steps





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Continuum Digital Twin

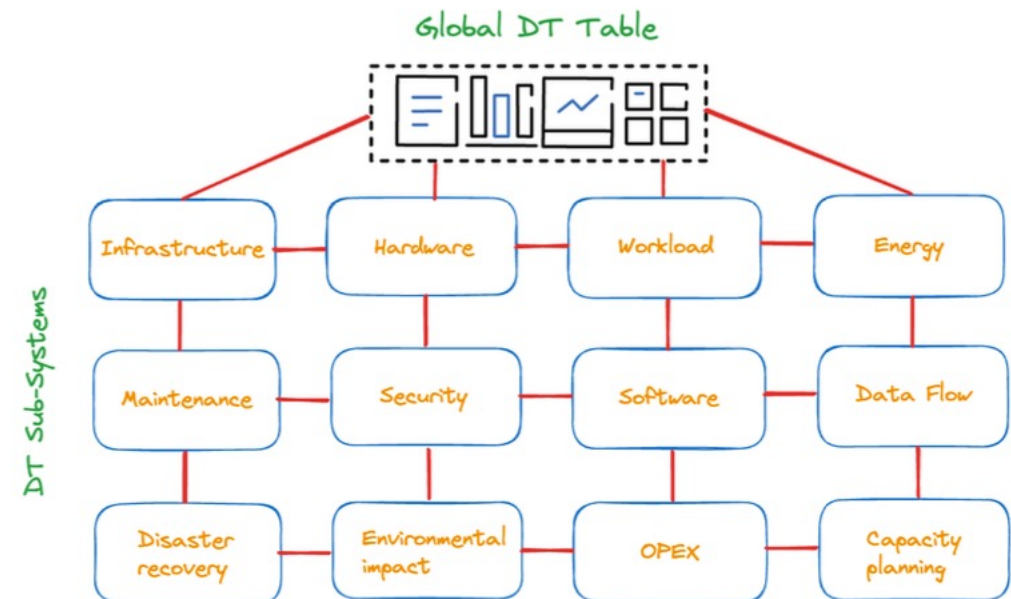
- The digital twin abstracts real systems to enable cross-facility workflows
- It operates without requiring direct interaction with physical infrastructure (cybersecurity constraints)
- Shares only essential information needed for orchestration, protecting sensitive aspects of the real infrastructure
- Facilitates real-time data flows from the infrastructure to the digital twin
- Ensures efficient and secure data exchange

Concrete Continuum Digital Twin

- A set of coupled microservices
- A formal model combining
 - Space-state
 - Constraints

$$X_k = A_{k-1}X_{k-1} + B_k u_k + w_k,$$

$$Y_k = C_k X_k + v_k,$$





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DDF Experiment Mathis Certenais

Objectives of the experiments



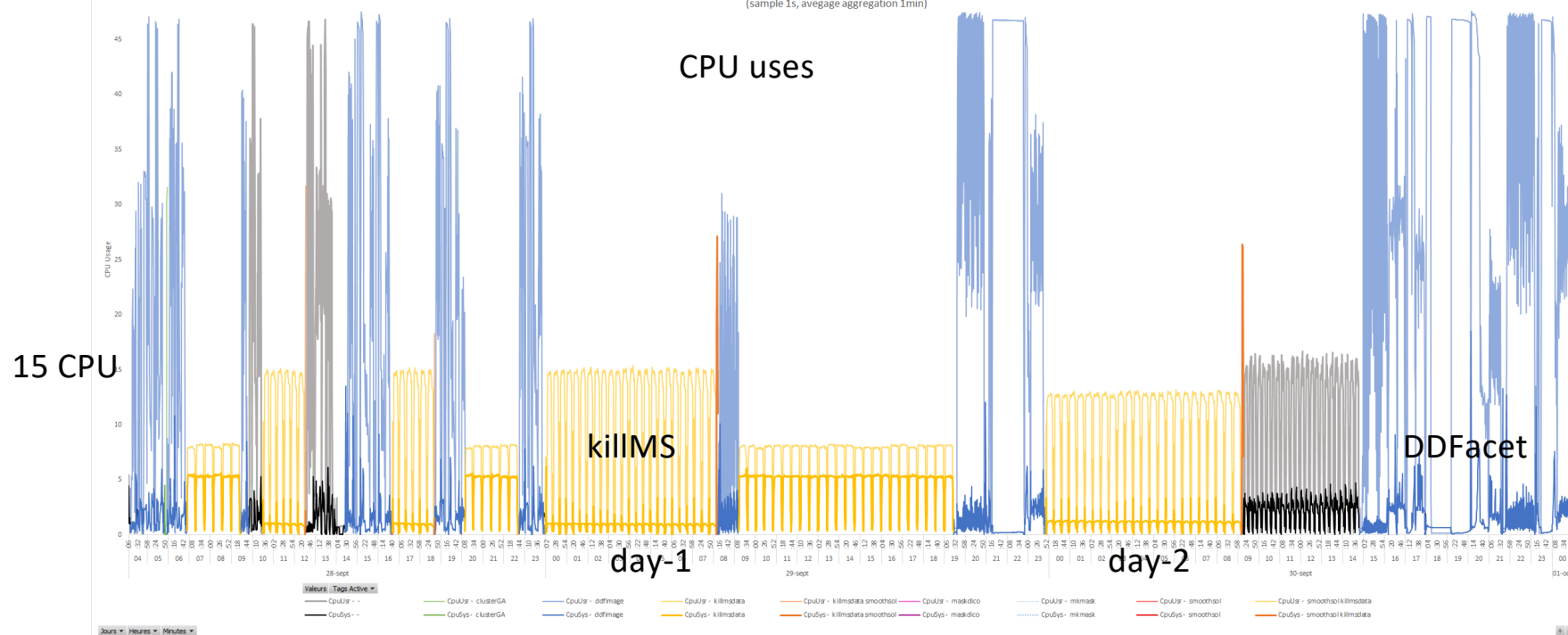
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- Evaluate global Exa-AToW architecture and propose solution for a first implementation
 1. Support use case based on DDF Pipeline
 2. Agent-based simulation, ILP-based optimization
 3. Study large-scale workflows deployment
 4. Propose data logistics based on the Cybercosm concept
 1. Avoid large scale distributed storage
 2. Ephemeral buffer based data transfers
 3. Interoperability as a main property

Execution profiling

50 CPU



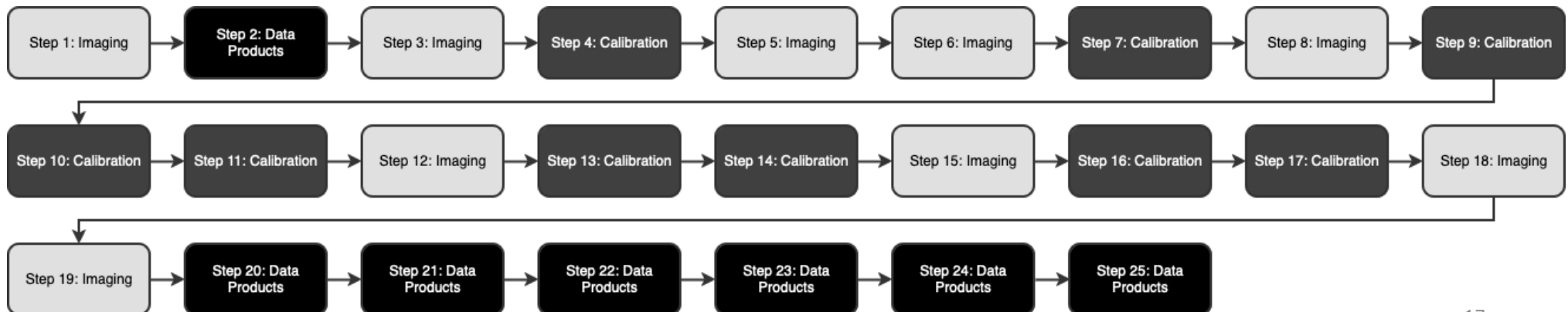
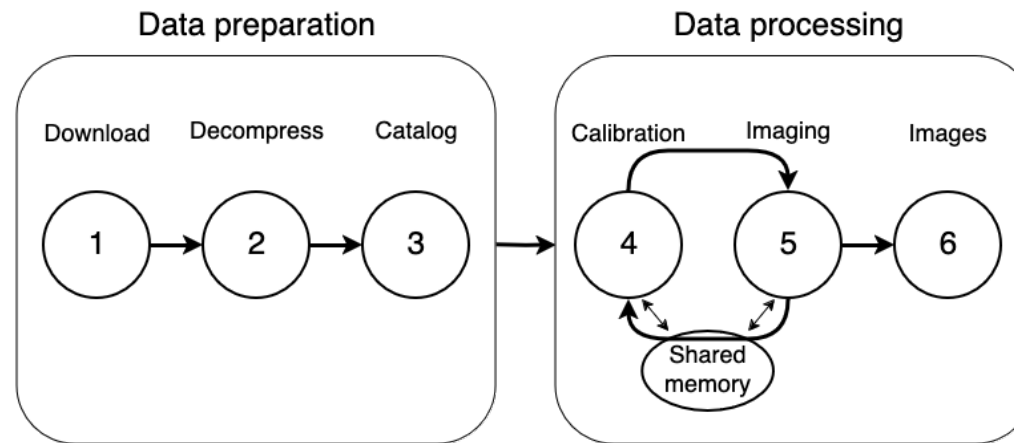
Process name	Cpu Usr	Cpu Sys	Dsk/#Total Read	Dsk/#Total Writ	MemUsed (Gbytes)	MemCached (Gbytes)
ddfimage	25,1	1,5	5488,3	13034,0	45,7	428,5
no profile	12,3	1,9	68923,8	6335,8	37,4	425,2
killmsdata smoothsol	10,9	12,0	63353,5	618,8	13,6	382,6
killmsdata	9,2	2,5	11641,1	18397,8	33,6	414,4
clusterGA	5,5	0,7	125542,0	10711,4	14,1	384,4
maskdico	0,7	0,1	294100,9	15248,5	13,0	376,5
smoothsol	0,7	0,1	1241088,0	0,0	11,7	354,4
mkmask	0,5	0,7	647272,4	55726,5	14,8	388,3

Eskemm single node – 120 CPU, 396 GB RAM
75h global run, 69h for processing, 37h killMS process, 23h DDFacet process.
Node spec: 2 x AMD EPYC 7543 32-Core Processor, 32 cores, 2.8GHz

Pipeline architecture



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From pipeline to workflow

