



eFlows4HPC

Introduction to the eFlows4HPC software stack and HPC Workflows as a Service methodology

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ISC-HPC, Hamburg May 21st, 2023



This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway. MCIN/AEI/10.13039/501100011033 and the European Union NextGenerationEU/PRTR (PCI2021-121957)

Agenda



9:00 – 9:15	Overview of eFlows4HPC project and tutorial agenda	Rosa M Badia (BSC)
9:15 - 9:35	Part 1.1: Integrating different computations in PyCOMPSs	Rosa M Badia (BSC)
9:35 – 10:05	Part 1.2: HPC ready container images	Jorge Ejarque (BSC)
10:05 - 10:35	Part 1.3: Data Pipelines and Data Logistics Service (DLS)	Jedrzej Rybicki (JSC)
10:35 - 10:55	Part 1.4: TOSCA Orchestration and HPCWaas	Jorge Ejarque (BSC)
10:55 – 11:00	Conclusion of part 1	Rosa M Badia (BSC)
11:00 - 11:30	Coffee break	
11:30 - 12:05	Part 2.1: Hands-on session: How to build HPC Ready containers	Jorge Ejarque (BSC)
12:05 - 12:30	Part 2.2: Hands-on session: How to move data with the DLS	Jedrzej Rybicki (JSC)
12:30 - 12:45	Part 2.3: Video demonstrating deployment with Allien4Cloud	
12:45 - 13:00	Tutorial conclusions	all presenters

Slides and other material available in https://github.com/eflows4hpc/ISC23_tutorial

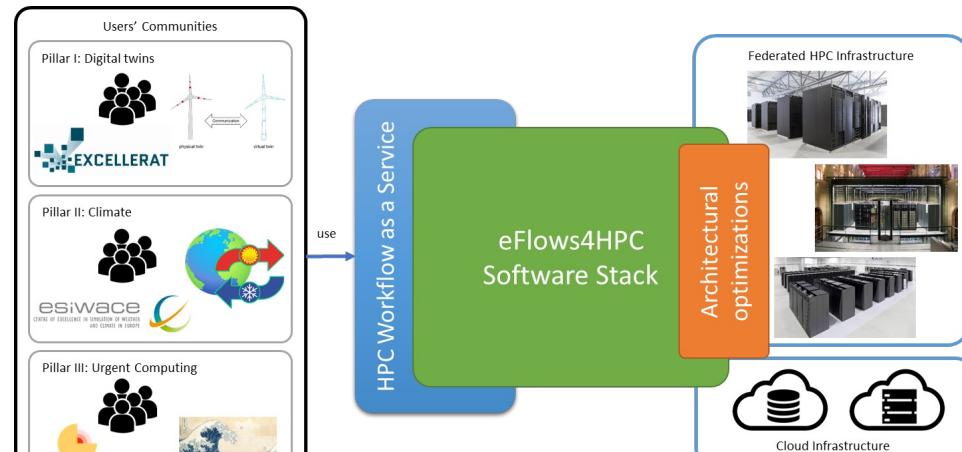


OVERVIEW OF EFLOWS4HPC

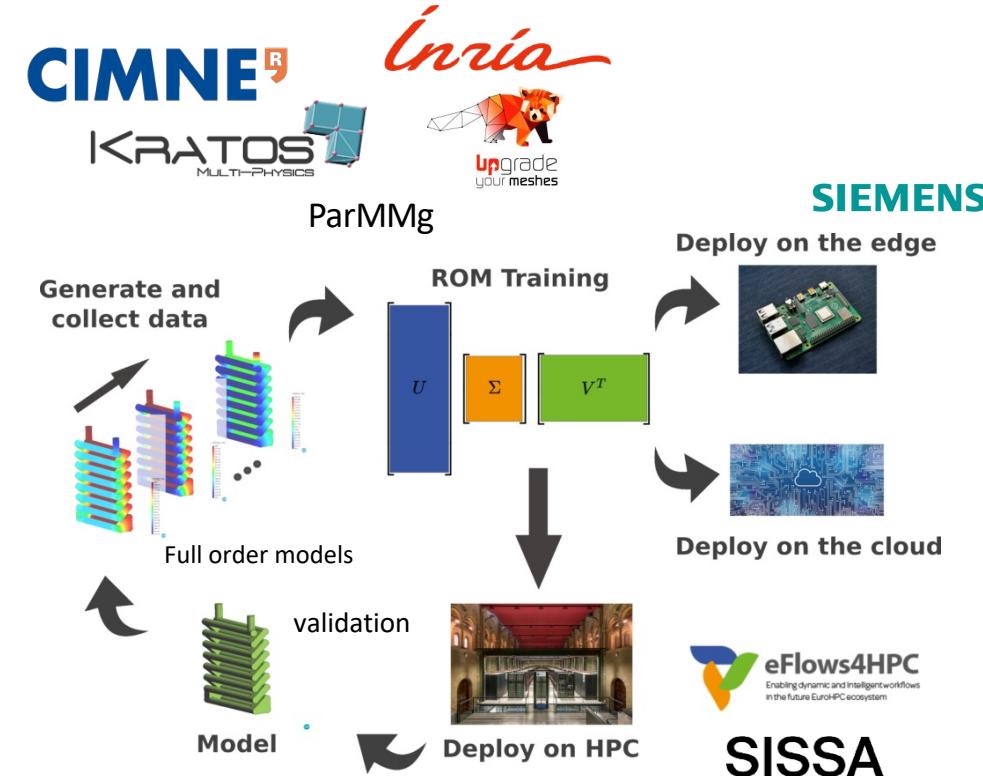
eFlows4HPC in a nutshell



- **Software tools stack that makes easier the development and management of complex workflows:**
 - Combine different frameworks
 - HPC, AI, data analytics
 - Reactive and dynamic workflows
 - Autonomous workflow steering
 - Full lifecycle management
 - Not just execution
 - Data logistics and Deployment
- **HPC Workflows as a Service:**
 - Mechanisms to make easier the use and reuse of HPC by wider communities
- **Architectural Optimizations:**
 - Selected HPC – AI Kernels Optimized for GPUs, FPGA, EPI
- **Validation Pillar's**
 - End-user workflows linked to CoEs

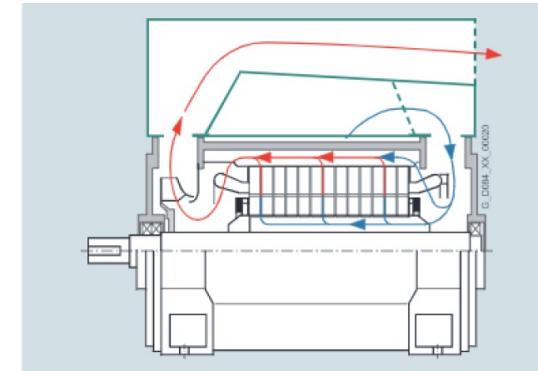


Pillar I: Manufacturing

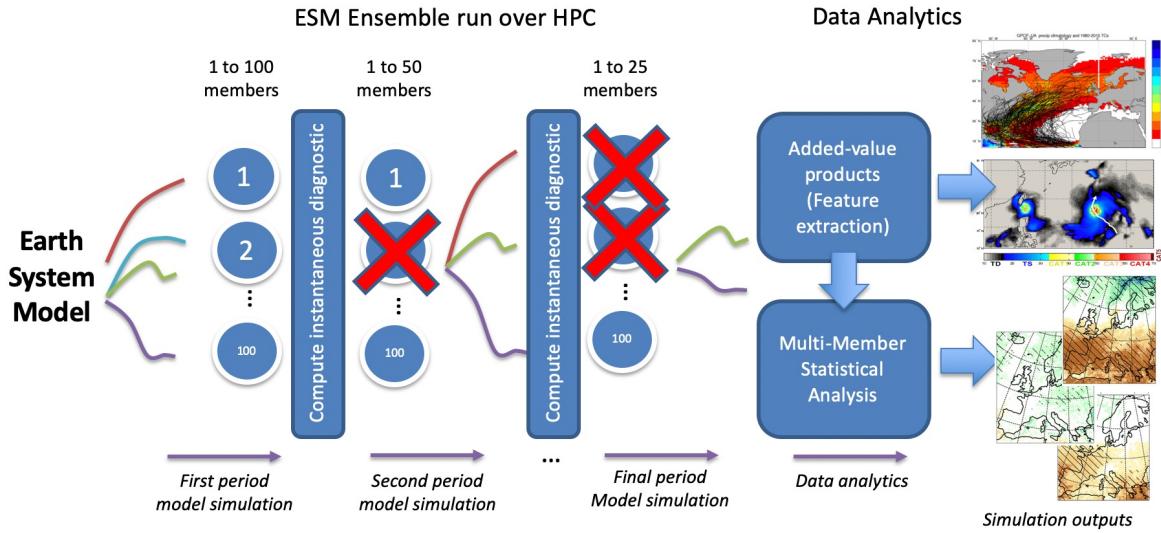


Pillar I focuses on the construction of Digital Twins for the prototyping of complex manufactured objects:

- Integrating state-of-the-art adaptive solvers with machine learning and data-mining
- Contributing to the Industry 4.0 vision



Pillar II: Climate



Dynamic (AI-assisted) workflow



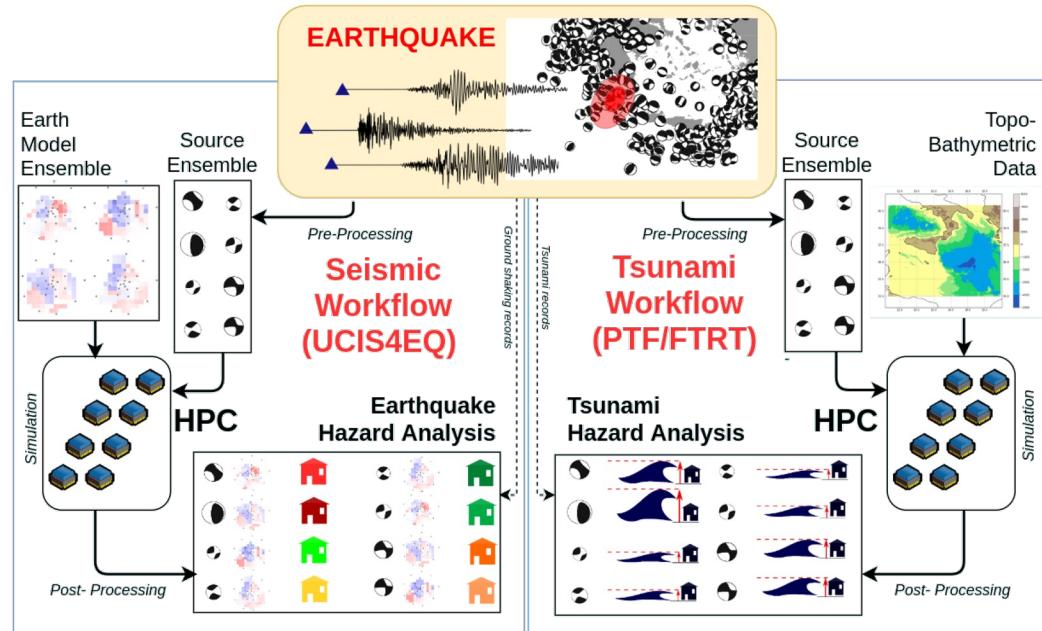
FESOM2
Finite volume Sea Ice-Ocean Model



HPDA & ML/DL

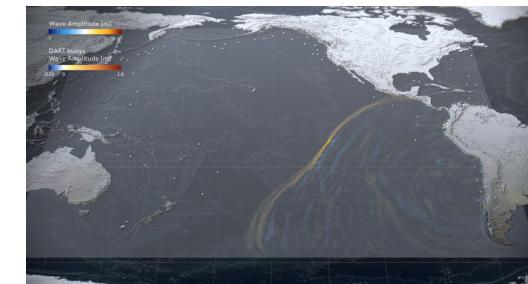
- Perform climate predictions: temperature, precipitation or wind speed
- AI-assisted pruning of the ESM workflow
- Study of Tropical Cyclones (TC) in the North Pacific, with in-situ analytics

Pillar III: Urgent computing for natural hazards



Pillar III explores the modelling of natural catastrophes:

- Earthquakes and their associated tsunamis shortly after such an event is recorded
- Use of AI to estimate intensity maps
- Use of DA and AI tools to enhance event diagnostics
- Areas: Mediterranean basin, Mexico, Iceland and Chile



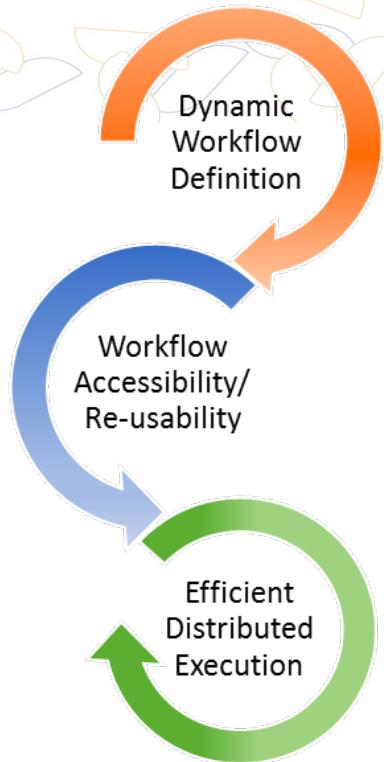
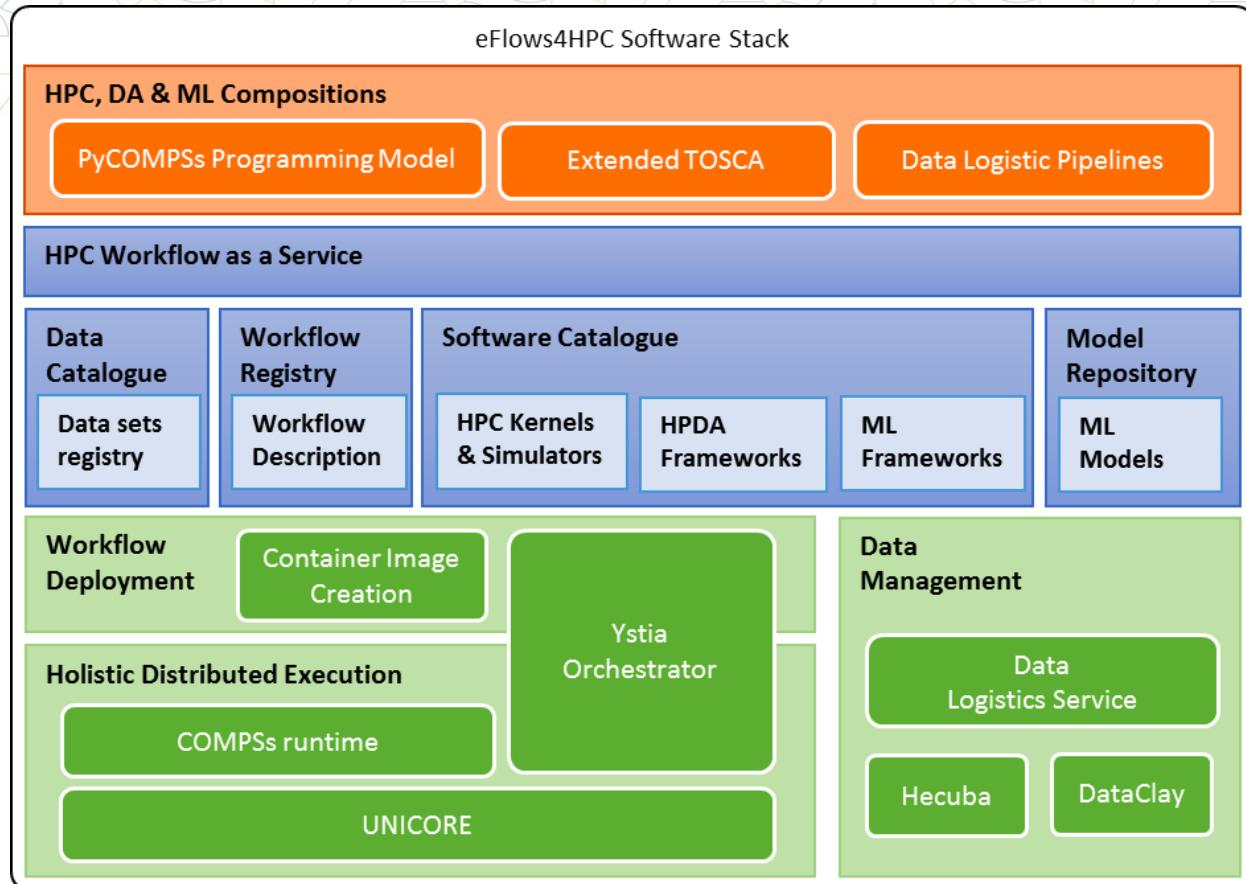
Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación

ETH zürich

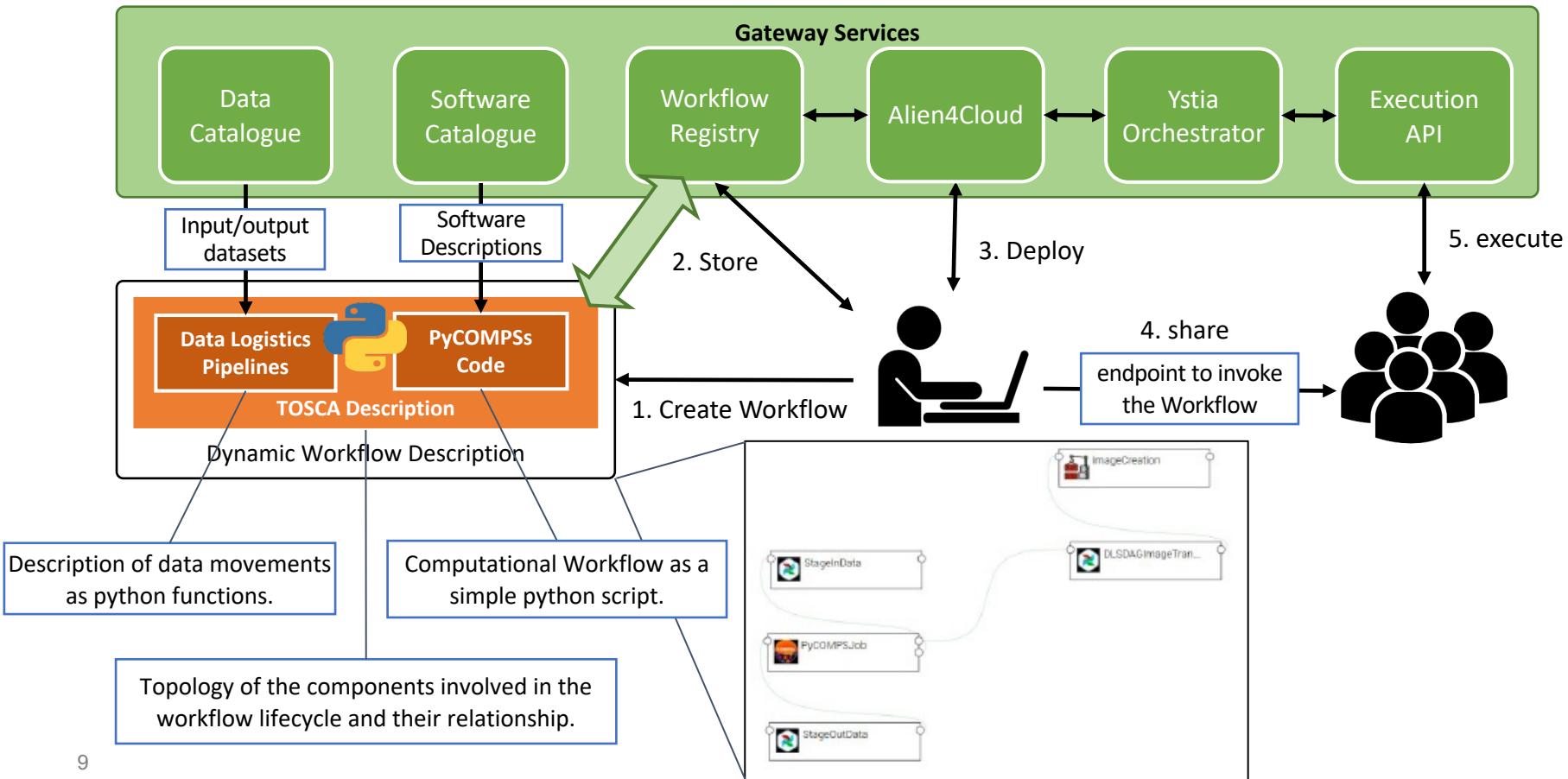


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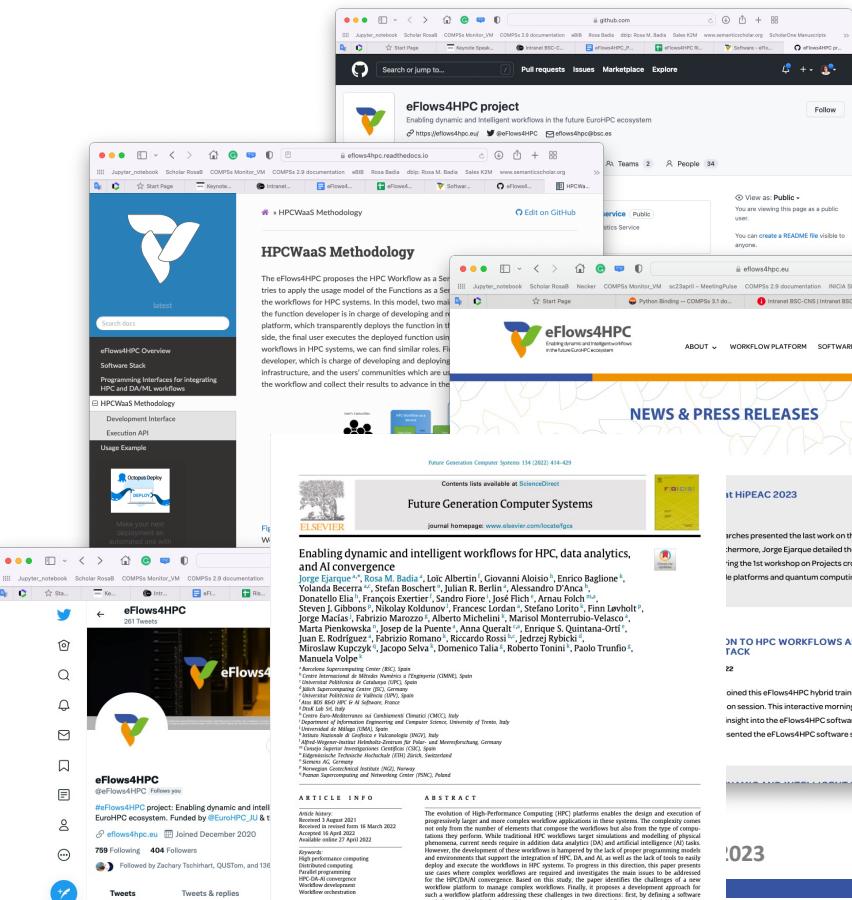


HPCWaas Overview



Project achievements

- Requirements and software architecture. Reviewed at beginning of second iteration
- Definition and implementation of abstractions to support the integration of different stack components
- Design and development of a minimal workflow. Development of a step-by-step example.
- Design and implementation of the HPCWaaS API
- Design and implementation of project services: Data Catalogue, Workflow Registry, Software catalogue
- Design and implementation of first version of Pillars' workflows.
- Two releases of project software and documentation available
- Set of internal trainings about software stack components and HPCWaaS. ICS-HPC tutorial
- Good visibility: articles, keynote presentations, media



The image displays several screenshots of the eFlows4HPC GitHub repository and its associated website. The top screenshot shows the GitHub repository page with the repository name "eFlows4HPC project" and a brief description: "Enabling dynamic and intelligent workflows in the future EuroHPC ecosystem". Below this are three screenshots of the eFlows4HPC website. The leftmost screenshot shows the homepage with sections for "eFlows4HPC Overview", "Software Stack", "Programming Interfaces for integrating HPC and Data/ML workflows", "HPCWaaS Methodology", "Development Interface", "Execution API", and "Usage Example". The middle screenshot shows the "HPCWaaS Methodology" page, which includes a detailed description of the methodology and a screenshot of a workflow interface. The rightmost screenshot shows the "NEWS & PRESS RELEASES" section, featuring a news item from "Future Generation Computer Systems 134 (2022) 414-429" and a press release from "eFlows4HPC: Enabling dynamic and intelligent workflows in the future EuroHPC ecosystem". At the bottom, there is a list of acknowledgments and a section titled "ARTICLE INFO" with a detailed abstract.

Tutorial focus (I): HPC Workflows as a Service methodology

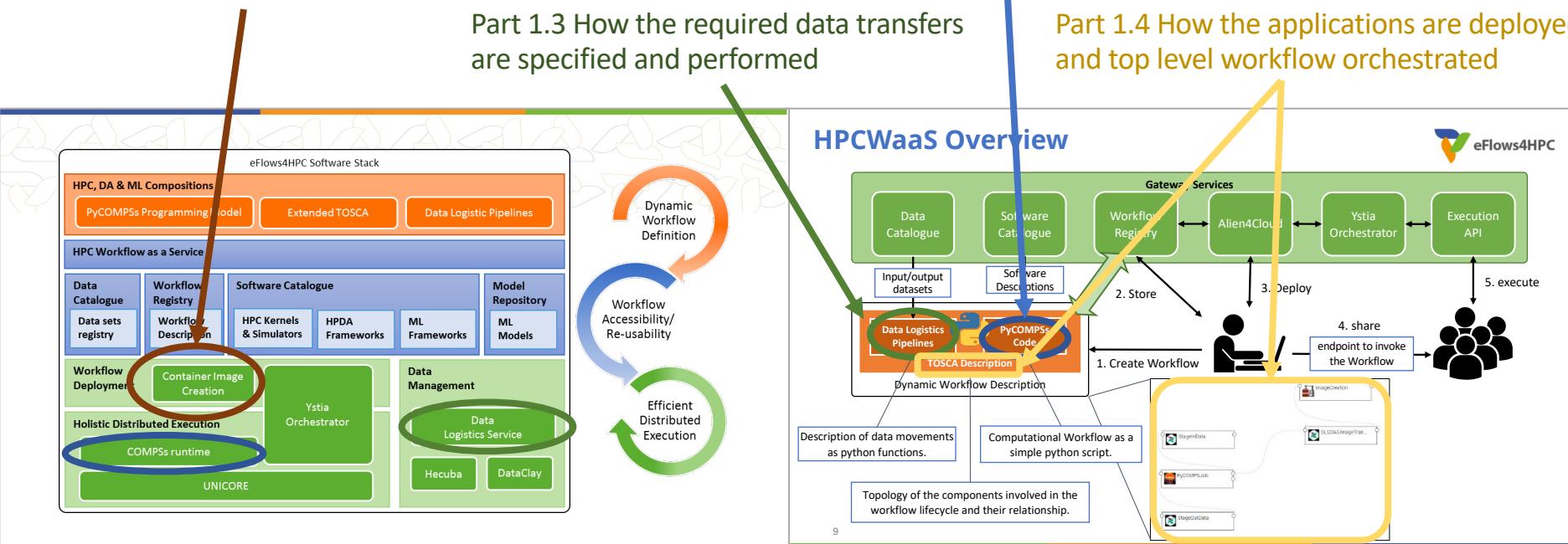


Part 1.2 How to generate HPC specialized containers

Part 1.3 How the required data transfers are specified and performed

Part 1.1 How different type of computations (HPC modelling and simulation, artificial intelligence and data analytics) are combined

Part 1.4 How the applications are deployed and top level workflow orchestrated



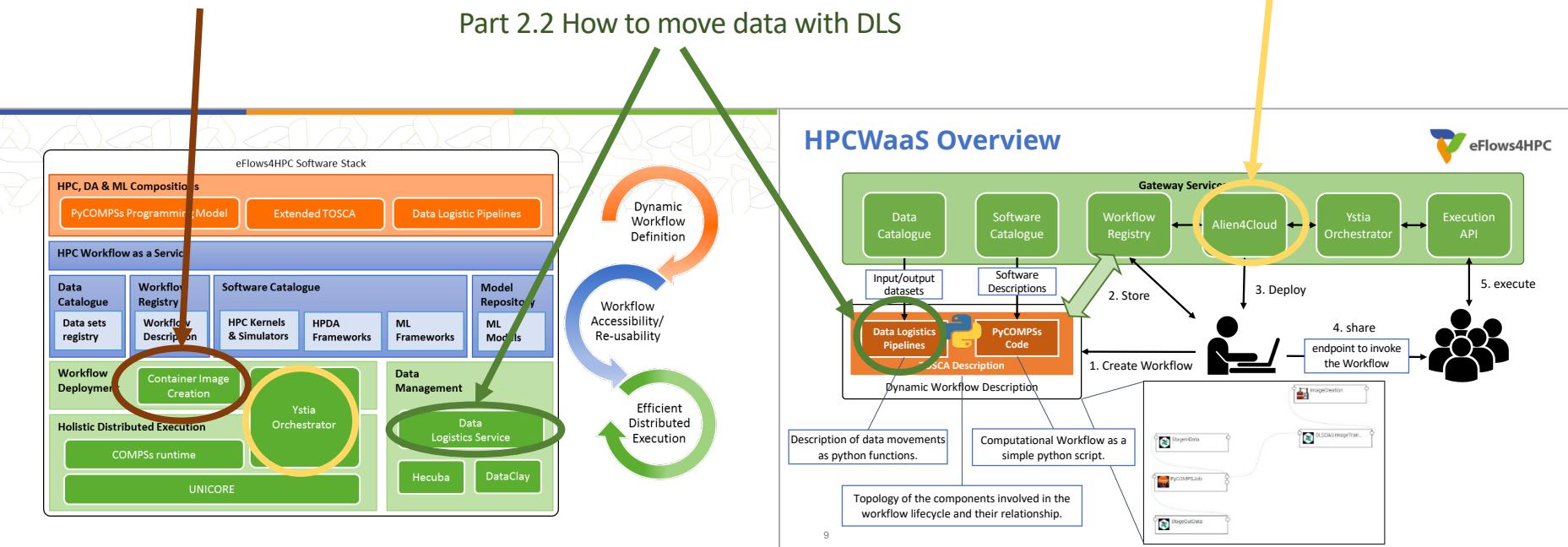
Tutorial focus (II): HPC Workflows as a Service methodology



Part 2.1 How to built HPC Ready containers

Part 2.2 How to move data with DLS

Part 2.3 How to deploy applications with Alien4Cloud



Project partners





eFlows4HPC

Enabling dynamic and Intelligent workflows
in the future EuroHPC ecosystem

www.eFlows4HPC.eu



@eFlows4HPC



eFlows4HPC Project



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