LEXIS Weather and Climate Large-Scale Pilot

Antonio Parodi[1(✉)], Emanuele Danovaro[2], James Hawkes[2], Tiago Quintino[2], Martina Lagasio[1], Fabio Delogu[1], Mirko D'Andrea[1], Andrea Parodi[1], Biagio Massimo Sardo[1], Andrea Ajmar[3], Paola Mazzoglio[3], Fabien Brocheton[4], Laurent Ganne[5], Rubén J. García-Hernández[6], Stephan Hachinger[6], Mohamad Hayek[6], Olivier Terzo[7], Jan Krenek[8], and Jan Martinovic[8]

[1] CIMA Research Foundation, Savona, Italy
antonio.parodi@cimafoundation.org
[2] ECMWF, Reading, UK
[3] ITHACA-POLITO, Turin, Italy
[4] NUMTECH, Aubière, France
[5] ATOS/BULL, Grenoble, France
[6] LRZ, Garching, Germany
[7] LINKS Foundation, Turin, Italy
[8] IT4Innovations, VSB – Technical University of Ostrava, Ostrava, Czech Republic

Abstract. The LEXIS Weather and Climate Large-scale Pilot will deliver a system for prediction of water-food-energy nexus phenomena and their associated socio-economic impacts. The system will be based on multiple model layers chained together, namely global weather and climate models, high-resolution regional weather models, domain-specific application models (such as hydrological, forest fire risk forecasts), impact models providing information for key decision and policy makers (such as air quality, agriculture crop production, and extreme rainfall detection for flood mapping). This paper will report about the first results of this pilot in terms of serving model output data and products with Cloud and High Performance Data Analytics (HPDA) environments, on top a Weather Climate Data APIs (ECMWF), as well as the porting of models on the LEXIS Infrastructure via different virtualization strategies (virtual machine and containers).

Keywords: Hydro-meteorology · Data assimilation · High-performance computing · Cloud computing

1 Introduction

The H2020 Large-scale Execution for Industry and Society (LEXIS) project will design and develop an advanced engineering platform at the confluence of HPC, Cloud and Big Data which will leverage large-scale geographically-distributed resources from existing HPC infrastructure, employ Big Data analytics solutions and augment them with Cloud services. LEXIS project is built on the convergence of large-scale HPC and cloud-run data analytics workflows. The emphasis of LEXIS is on the interaction between HPC and cloud systems, built on top of data sharing and methods to compose workflows of tasks running on both cloud and HPC systems. LEXIS is developing platform to

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enable these workflows and demonstrate its abilities through three large-scale socio-economic pilots, targeting aeronautics, weather climate, and catastrophe alert systems. This paper reports the initial results concerning the Weather and Climate pilot which fully benefits of the project ongoing results in terms of orchestration system, distributed data infrastructure (DDI), and workflows orchestration.

2 The Weather and Climate Pilot

The Weather and Climate pilot focuses on a complex system, to provide a diverse set of forecasts concerning weather, flood, forest fire, air pollution and agriculture. The Weather and Climate pilot encompasses several complex workflows each consisting of various meteorological components. These workflows include ingestion of conventional and unconventional observations, global weather models, regional weather models, application models and socio-economic impact models (Fig. 1). These workflows will be run across disjoint computing resources. Global weather models will run on ECMWF's HPC in the UK; whilst regional weather models will run on HPCs in Italy (CIMA), Germany (LRZ) or Czechia (IT4I). Following this, application models and socio-economic impact models will be run on cloud-based resources in Germany or Czechia.

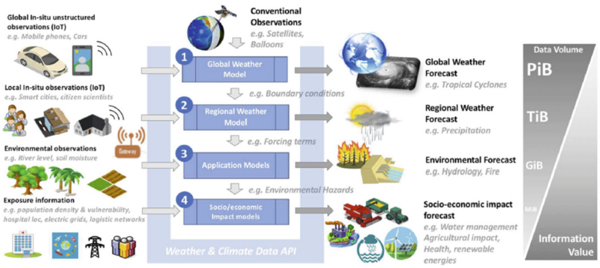

Fig. 1. LEXIS Weather and Climate complex workflows description.

Modelling Tasks
LEXIS is offering several weather and climate modelling tasks, as summarized in the following:

- The Weather Research and Forecasting (WRF) Model is a proven mesoscale numerical weather prediction system, designed to serve both operational forecasting and atmospheric research needs [12]. It features multiple dynamical cores, a 3-dimensional variational (3DVAR) data assimilation system [7,8], and a software architecture allowing for computational parallelism and system extensibility. WRF is suitable for a broad spectrum of applications across scales ranging from meters to thousands of kilometres.
- RISICO (RISchio Incendi e COordinamento/Fire Risk and Coordination) is a mathematical model developed by the CIMA Research Foundation [4] to support operators in forest fire prevention activities. RISICO is powered by a continuous data

flow consisting of meteorological information in real-time using both the weather forecast and satellite records. This information takes into account parameters such as the moisture content of the vegetation, the wind and the orography of the territory and allow to quantitatively assess the danger resulting from the eventual triggering of a forest fire both in terms of propagation speed and linear intensity of the flame front;

- Continuum is a hydrological model developed by the CIMA Research Foundation [14] to reproduce the flow of water within a basin, i.e. how much water passes into a given section of a river or a lake. Continuum is able to work both in the pre-event analysis and forecast phase and in the monitoring stage for the active control of hydrological events. The model has a reduced number of parameters and is also able to take advantage of all the information available via satellite;
- ADMS (Atmospheric Dispersion Modelling System) models [2,15] are managed by NUMTECH to perform atmospheric dispersion calculation depending of meteorological conditions and emission release. Two applications are performed: (i) industrial ones in order to forecast SO_2 impact at ground from industrial release in order to prevent pollution peak, and (ii) urban ones in order to forecast at high-scale NO_2 and PM concentration over a full city (Paris);
- The Extreme Rainfall Detection System (ERDS), developed and implemented by ITHACA [10], is a demonstration service for the monitoring and forecasting of exceptional rainfall events, with a nearly global spatial coverage. The information is accessible through a WebGIS application, developed in a complete Open Source environment. The system has been designed for the monitoring and forecasting of exceptional rainfall events. More importantly, the system is able to provide alerts about heavy rainfall events, flash floods, convective storms, tropical storms, cyclones and hurricanes.

Observational Data
Different observational dataset will be considered in this pilot:

- ECOMET dataset containing about 3000 authoritative weather stations. The data are provided for free for hindcast research studies. The data are available in BUFR format. The main usage will be the assimilation in the WRF model;
- CIMA has developed a partnership with IBM for about 150000 personal weather stations (PWS) real-time (hourly reporting temperature, wind, rainfall, relative humidity, pressure) over the globe (32000 from Europe, Fig. 2). Also, historical data will be available for 1 June – 30 November 2018 (about 13000 personal weather stations from Europe). The main usage will be the assimilation in the WRF model.
- Italian Civil Protection Department (ICPD) dataset: The Italian Civil Protection Department is designing and managing in real time risk reduction actions over the national territory, determined by high-impact adverse weather, through its Centro Funzionale Centrale (Central Functional Center), and coordinating a federated national Early Warning System, in collaboration with regional authorities. In this framework, ICPD manages a large number of in-situ authoritative weather stations: 6,059 rain gauges, 2299 hydrometers, 4373 thermometers, 1270 barometers, about 2500 anemometers, and finally 2,683 hygrometers. The data temporal resolution is

approximately 1 min. CIMA archives and curates the aforementioned data on behalf of ICPD.

- ICPD and MeteoFrance radar dataset: for the period 1 June – 30 November 2018 reflectivity radar CAPPI (500 m vertical resolution over 500–12,000 m, 2.5×2.5 km grid spacing) over the France territory at large. Provided in ASCII format to be stored on CIMA storage services, this data will be assimilated in the CIMA WRF regional forecast. For the years 2018 and 2019, reflectivity radar CAPPI (2,000–3,000–5,000 m, 2 km $\times$ 2 km grid spacing) over the Italian territory at large, in NetCDF format. These data will be assimilated in the CIMA WRF regional forecast.
- Integrated Multi-satellitE Retrievals: The Integrated Multi- satellitE Retrievals for GPM (IMERG, [6]) is the unified U.S. algorithm that provides the Day-1 multi-satellite precipitation product for the U.S. GPM team. The precipitation estimates from the various precipitation-relevant satellite passive microwave (PMW) sensors comprising the GPM constellation are computed using the 2014 version of the Goddard Profiling Algorithm, then gridded, intercalibrated to the GPM Combined Instrument product, and combined into half-hourly $0.1 \times 0.1^\circ$ fields. Original data are provided in HDF5 and GeoTIFF file format through FTP and OPeNDAP service.

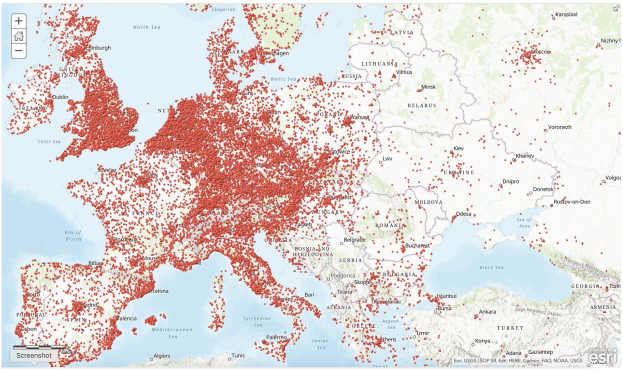

Fig. 2. Weather Underground european weather stations network.

3 LEXIS Distributed Data Infrastructure and Weather and Climate Data API

The LEXIS "Distributed Data Infrastructure" (DDI) is based on an *iRODS*[1] data management system with fault-tolerant setup. This integrates seamlessly with the services *B2SAFE*, *B2STAGE* and *B2HANDLE* of the European Collaborative Data Infrastructure EUDAT[2]. The *iRODS* back-end is organized in federated zones (one per supercomputing centre); this allows users to access their data independently of its actual location, and to request automatic replication and migration of data on an as-needed basis.

[1] https://irods.org/.
[2] https://eudat.eu/.

Modern JSON-based REST APIs have been designed and implanted as a frontend to the iRODS backend, enabling upload, download and deletion of datasets, managing of access rights and staging of data sets into computational resources. Datasets are accompanied by relevant metadata, so that data can be findable according to FAIR principles. Asynchronous transfers are implemented as a consequence of the data volumes involved in LEXIS; an appropriate queuing system allows the user to follow the progress of their requests. The DDI is secured using the global LEXIS Authentication and Authorisation (AAI) infrastructure, which it interfaces to via OpenID[3]. The LEXIS AAI is based on via *Keycloak*[4] instances. The setup uses token hashing to allow *iRODS* and *Keycloak* to interact [5].

However, the LEXIS DDI does not exist in a vacuum: some data sets required for the Weather and Climate Large-scale Pilot have been stored (and continue to be stored) in previously-developed domain-specific storage libraries. These systems can often provide a more feature-rich view of the data sets, due to their domain knowledge. In addition, legacy hard- and software systems continue to access these libraries for up- and downloading observations, sometimes even in near-real-time.

In order to provide a state-of-the-art domain-specific storage library for curated weather and climate data, the LEXIS project implements the "Weather and Climate Data API" (WCDA). It is responsible for storing and organizing weather observations from a variety of sources (including in-situ unstructured observations), as well as numerical weather prediction outputs and intermediate weather data. Data are indexed according to domain-specific metadata, to efficiently support metadata-based queries. Additionally, WCDA has been designed to provide efficient distributed access to ECMWF's MARS, to our knowledge the largest European meteorological archive. MARS stores more than 300 PB of meteorological and climatological data, from observations to global model outputs. Internally, WCDA utilises a via *FDB* object store, which provides indexing capabilities and support for different storage systems (parallel FS, Ceph cluster). Each instance of WCDA can provide seamless access to local and remote data by contacting other WCDA instances available on the LEXIS platform. The WCDA interface is RESTful and the backend is based on a fully scalable architecture with containerized components. It can be deployed with Docker Compose or in a Kubernetes cluster.

The Weather and Climate Large-scale pilot has thus two data infrastructures it can rely on – the specialised WCDA for efficient handling of meteorological data, and the DDI which facilitates data exchange as well as general-purpose sharing and publications of results. The usage of both systems will be combined for maximum efficiency.

4 YORC and HEAppE in the LEXIS Orchestration System

The LEXIS Platform, with its Hybrid HPC/Cloud systems in the backend, uses an orchestration system for workflows (sequences of operations on application components) to be executed. The applications to be deployed are modeled using the Topology and Orchestration Specification for Cloud Applications (TOSCA, [1]), an OASIS

[3] https://openid.net/.

[4] https://www.keycloak.org/.

consortium standard language to describe an application made of components, with their relationships, requirements, capabilities, and operations. Workflow orchestration, execution and monitoring in LEXIS is based on *Yorc*[5] (Ystia orchestrator, including Alien4Cloud and other components) and *HEAppE*[6] [16] (High-End Application Execution Middleware). We have developed the *Yorc HEAppE plugin*, which extends the Ystia Orchestrator (*Yorc*) so it can use *HEAppE* as middleware.

Yorc is our solution for high-level orchestration of workflows. Its front-end, Alien4Cloud, provides a studio allowing to create applications from an extensible catalog of TOSCA components, deploy these applications, run and monitor workflows.

The *HEAppE* middleware is an application framework developed to allow average users to run complex calculations on HPC infrastructure via the user interface of a client application, without the necessity to connect directly to the HPC cluster. HEAppE is able to provide information about the status of submitted jobs and to ensure data transfer between HPC infrastructure and a client-side app. HEAppE also provides a mapping of LEXIS user identities to the user accounts on HPC systems. The HPC-centre account to which the LEXIS user is mapped is a particular (functional account usually not personalised) account associated with an HPC project Id as per approval of the project's principal investigator (PI). For this mapping and the HEAppE mechanism to work, the project PI need does not have any affiliation with LEXIS whatsoever [16].

For each modelling task of our Weather and Climate Large-scale Pilot workflow, the LEXIS Orchestration System can dynamically select available and appropriate computing resources from all LEXIS sites. This approach allows each of the modelling tasks to execute as fast as possible, and integration with different European computing centres increases redundancy for a reliable execution. To benefit from all this, it is essential to have task implementations ready for all the relevant computing resources. The Weather and Climate Large-scale Pilot workflow implementation includes a set of tasks for Cloud as well as HPC systems in LEXIS. The workflow is thus ideally suited for execution on the hybrid platform.

The proposed orchestration system solution features an open and user-friendly design, aimed at maximum compatibility. This not only minimises the effort for porting Pilots and other users' workflows to the LEXIS platform, but also facilitates a future integration of more computing and data centres with LEXIS.

5 Weather and Climate Pilot Workflows

The LEXIS Weather and Climate Large-scale Pilot includes aforementioned numerical modelling tasks from weather prediction to hydrological prediction, forest fire risk forecast, air quality and industrial pollution forecasting, as well as extreme rainfall detection system.

Concerning the *hydrological prediction*, building also on top of the FP7 Distributed Research Infrastructure for Hydro-Meteorology (DRIHM) results [11], the complete workflow involves different LEXIS tasks such as the meteorological model WRF, including a WRFDA data assimilation system and the fully distributed hydrological

[5] Yorc: https://github.com/ystia/yorc.

[6] HEAppE Middleware: http://heappe.eu.

model Continuum (Fig. 3), which have already demonstrated their combined potential in research activities [8]. The WRF model is executed as a task on high performance computing facilities (HPC capabilities at IT4I & LRZ) after the preparation of initial and boundary conditions provided by the WRF Preprocessing System WPS. The WPS task is executed, as container[7], on cloud computing facilities (LRZ and IT4I) and it allows processing ECMWF (European Centre for Medium-Range Weather Forecasts) IFS (Integrated Forecasting System) and NCEP (National Centers for Environmental Prediction) GFS (Global Forecast System) global circulation model data to generate input fields for the WRF model itself. The WRFDA task is a flexible, state-of-the-art atmospheric data assimilation system that is portable and efficient on available parallel computing platforms: WRFDA is a task executed on cloud computing facilities (HPC capabilities at IT4I & LRZ). The Continuum hydrological model is executed as sequential task (container[8]) on cloud computing facilities (HPC capabilities at IT4I & LRZ). The results of the hydrological prediction workflow will be published on the MyDewetra platform [3], a web-based real-time system for hydro-meteorological forecasting and monitoring developed by CIMA on behalf of the Italian Civil Protection Department.

Concerning the *forest fire risk prediction*, the complete workflow involves the aforementioned meteorological task WRF, including the WRFDA data assimilation system, and the fire risk model RISICO (container[9], in place of the Continuum model in the hydrological workflow.

For the *air quality prediction*, the complete workflow involves the aforementioned meteorological task WRF, including the WRFDA data assimilation component, and the ADMS, in place of the Continuum model in the hydrological workflow.

Concerning the ERDS is a service for the *monitoring and forecasting of exceptional rainfall events*, with a nearly global geographic coverage. Available capabilities include the analysis of both the near real-time and the forecast rainfall amount for different lead times, with the aim to deliver extreme rainfall alerts. IMERG early run products, are downloaded as near real-time source of rainfall measurements. GPM IMERG data are characterized by a temporal resolution of 30 min, a $0.1 \times 0.1^\circ$ spatial resolution and a spatial coverage between 90° north and 90° south. The ERDS methodology is based on the concept of threshold: a threshold represents the amount of precipitation needed to trigger a flood event induced by extreme rainfall. Specifically, if for a selected aggregation interval the accumulated precipitation exceeds the threshold, an alert is provided. This set of thresholds has been calculated at a $1 \times 1^\circ$ spatial resolution for every aggregation interval on the basis of the mean annual precipitation that affects each place of Earth's surface. The mean annual precipitation was calculated using 10 years of GPCC monthly monitoring products. This system is also able to provide longer lead-time alerts (up to 4 days) for heavy rain, using forecast rainfall data coming from NOAA-GFS (Global Forecast System) deterministic weather prediction models, with a $0.25 \times 0.25^\circ$ spatial resolution and worldwide coverage, updated on a 12-h basis. Alerted areas can be exploited for the definition of specific Areas of Interest (i.e., areas particularly affected by heavy rainfall) that could be used as input for two different processes. The first one

7 https://github.com/cima-lexis/wps.docker.

8 https://github.com/cima-lexis/fp-docker.

9 https://github.com/cima-lexis/risico-docker.

involves the execution of higher resolution forecasting models over selected areas (not applicable over a global domain due to computational constraints) in urgent computing mode [9], such as the WRF model task of CIMA built of top of consolidated WRF modelling operational expertise[10]. The second one is the initiation of a Satellite Emergency Mapping (SEM) mechanism. The timely identification of the most affected areas is, in fact, a valuable aspect for the pro-active request of satellite images that will be used in the emergency map production. After the reception of the satellite images, a more precise identification of the flooded areas will be performed by means of a computer-aided photointerpretation.

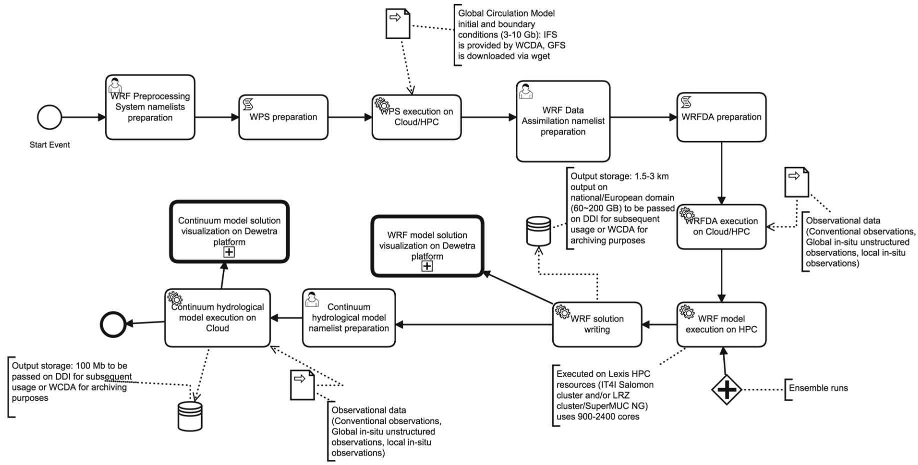

Fig. 3. LEXIS Weather and Climate complex workflows description.

6 Workflows Mapping on LEXIS Platform

The Weather and Climate Large-scale Pilot workflows components will be mapped as follows on the LEXIS platform:

- WRF model will be executed on HPC systems (LRZ and IT4I)
- Containers and virtual machines will be executed on cloud computing
- Workflows will be executed by the LEXIS Orchestration System (Sect. 4)
- DDI (Sect. 3) will support the data exchange between the Weather and Climate models

These TOSCA applications and associated workflows will be developed incrementally, integrating new features as they become available, like for example the use of LEXIS WCDA API to manage datasets [13]. Hereafter the TOSCA implementations of RISICO workflow is described for sake of clarification and description of the work developed at this stage by the LEXIS project. The RISICO workflow is implemented at it follows:

- Creating a Virtual Machine on LEXIS cloud
- Retrieving GFS model and Geographical data on this Virtual Machine
- Running the WRF Preprocessing System (WPS) container

[10] https://www.cimafoundation.org/foundations/research-development/wrf.html.

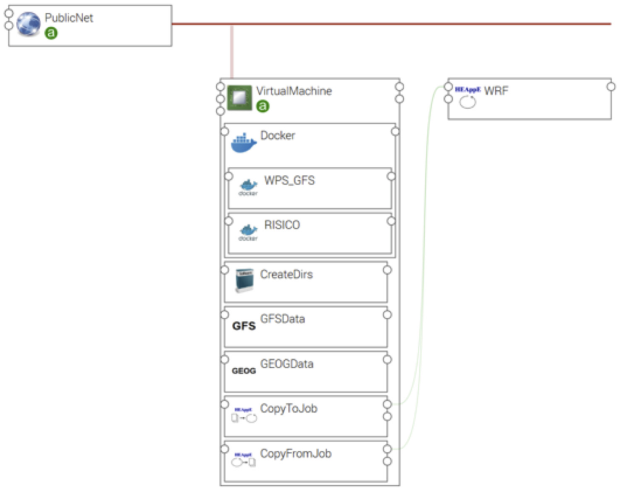

Fig. 4. Graphical view of the RISICO application template

- Submitting a WRF job on the HPC infrastructure
- Running the RISICO container once the WRF job has produced its result files

The graphical view of the RISICO application template (Fig. 4) shows the following components hosted on a Virtual Machine:

- Docker, to run containers
- WPS GFS, container performing the pre-processing
- RISICO, container performing the post-processing
- CreateDirs, component creating directories expected by containers
- GFSData component downloading Global Forecast System files from a web site
- GEOGData, component downloading geographical files from a web site
- CopyToJob, component copying pre-processing results to a Job input directory
- CopyFromJob, component copying Job computation results to the compute instance
- WRF HEAppE Job performing a computation on the HPC infrastructure

The associated workflow (Fig. 5) creates first a Virtual Machine, then downloads in parallel GFS and geographical data files. Docker is then installed on the Virtual Machine and the WPS GFS pre-processing container is run. Once done, the workflow goes on creating an HEAppE job on the HPC infrastructure (Fig. 6), the next step enables file transfers for this job. Then, the WPS GFS pre-processing results are copied to the job (component CopyToJob operation). The Job is then submitted, and the orchestrator waits until it ends. Once done, the Job results are copied to the Virtual Machine (component CopyFromJob operation). Finally, in parallel, the file transfer is disabled for the job and the job is deleted, while RISICO post-processing container is run.

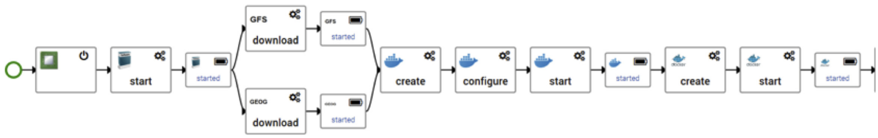

Fig. 5. RISICO workflow - part 1

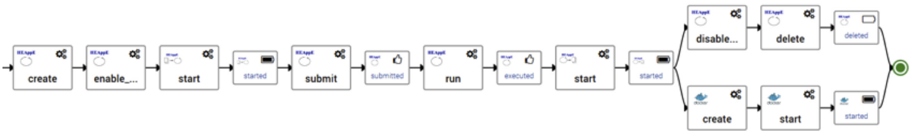

Fig. 6. RISICO workflow - part 2

7 Conclusions

This paper presented the first results of the LEXIS project concerning the formulation of next generation weather and climate Workflows. The LEXIS Distributed Data Infrastructure is described in detail in Sect. 3 as enabling element for the execution of LEXIS modelling tasks (Sect. 2). To the best of authors knowledge the YORC and HEAppE approaches are applied for first time to weather and climate modelling (Sect. 4) paving the way towards a more efficient execution of complex meteo-hydrological forecasting workflows. Next main step will be the testing of the current workflows on selected case studies and then the subsequent addition of the WRFDA modelling task as important element for subsequent production runs.

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