LEXIS PROJECT
LARGE-SCALE EXECUTION FOR INDUSTRY & SOCIETY

LEXIS Newsletter
March 2021

ICHEC and EURAXENT join the LEXIS project

We are pleased to announce that the LEXIS project has two new partners. The first partner is the Irish Centre for High-End Computing (ICHEC), which joined the LEXIS project for the platform validation phase. The second one is EURAXENT, led by Marc Derquennes, who will promote the Open Call of the LEXIS project.

Ireland's high-performance computing centre supports Ireland in realising the benefits of HPC, creating breakthroughs in science, economic development and evidence-based policies.

ICHEC provides expertise, training and support to local business and SMEs, supports academic researchers in Ireland and Europe, and works with government agencies and local authorities to translate data into knowledge. This means that they provide solutions to some of the toughest challenges across public, academic and enterprise sectors in Ireland.

ICHEC
Irish Centre for High-end Computing

EURAXENT

ICHEC operates from offices in National University of Ireland, Galway and Dublin City Centre employing more than 40 staff.

ICHEC supports researchers to bring new solutions to the complex scientific and social challenges of today, provides essential data analysis to Public Service Bodies and supports SMEs through optimising data challenges.

More information: www.ichec.ie

EURAXENT is the new partner organisation led by Marc Derquennes, the task leader of the LEXIS project for the Open Call and for exploitation. Marc has 30 years of experience at the crossroads of science, research, technology and operations management, leading the strategy and the development of technology companies and high-tech services.

More information: www.euraxent.com

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Latest News from LEXIS Open Call 2020–2021

CompBioMed collaborates with the LEXIS project in the Open Call

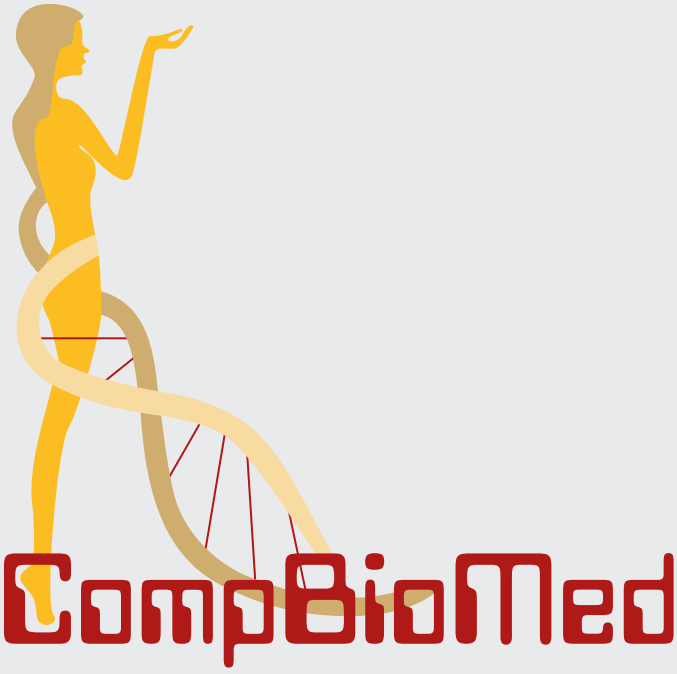
The CompBioMed Centre of Excellence has joined the Open Call of the LEXIS project, which is the starting point for a close collaboration. Thanks to the LEXIS platform, CompBioMed will transfer data more effectively and safely between computing centres. It can directly profit from the user-friendly and unified LEXIS approach to the usage of integrated HPC, Cloud and Edge resources with various computational techniques (Simulation, Big Data, AI) without expert knowledge. The collaboration will thus enable a broad range of users, from researchers to clinicians, to conveniently leverage and test multi-centre computing power for efficient biomedical computations.

For example, results of ensemble HPC simulations can be processed on remote machine learning clusters to construct the next generation of simulations. Ultimately, LEXIS helps CompBioMed to collate and share data securely. The consortium will support CompBioMed with the training, technical and scientific assistance to use and validate the LEXIS platform. This collaboration will be a good opportunity for both projects to share their experience, and the consortia are looking forward to working together.

LEXIS OPEN CALL
CompBioMed

CompBioMed Centre of Excellence

CompBioMed is a European Commission H2020 funded Centre of Excellence focused on the use and development of computational methods for biomedical applications. They have users within academia, industry and clinical environments and are working to train more people in the use of their products and methods. CompBioMed ran initially for 3 years from 2016 to 2019 and is now in its second project running for 4 years until 2023. The consortium consists of 16 core partners, 2 international partners and a growing team of over 50 associate partners. A great introduction to their project can be found in the Virtual Humans film (https://youtu.be/1FvRSJ9W734).



LEXIS Open Call Updates

The LEXIS project has launched its Open Call 2020–2021, for application experiments capable of exploiting and validating its powerful platform.

Started in December 2020, the call is open for applications until the end of June 2021. Selected application experiments can run until the end of November 2021.

To carry out the selection process, the Open Call committee meets once a month (next meeting: Thursday April 1, 2021).

LEXIS OPEN CALL

Who can submit?

- companies from the private sector (any size, any sector) including start-ups,
- academic institutions,
- research organizations, and
- other EU funded projects.

For more details, please check the LEXIS website and its Open Call pages.

" If you are interested in testing LEXIS platform, we recommend you to submit your projects as soon as possible & stay tuned! "

Before submitting your participation, please take your time to read the documentation made available online on our website.

To participate, please do the following:

1. Download the self-administered questionnaire.

2. Register your interest to the Open Call (no commitment) using the registration form and don't forget to subscribe to the LEXIS newsletter.

3. Check the open call's requirements and rules at Lexis website and its Open Call page.

4. Complete the questionnaire.

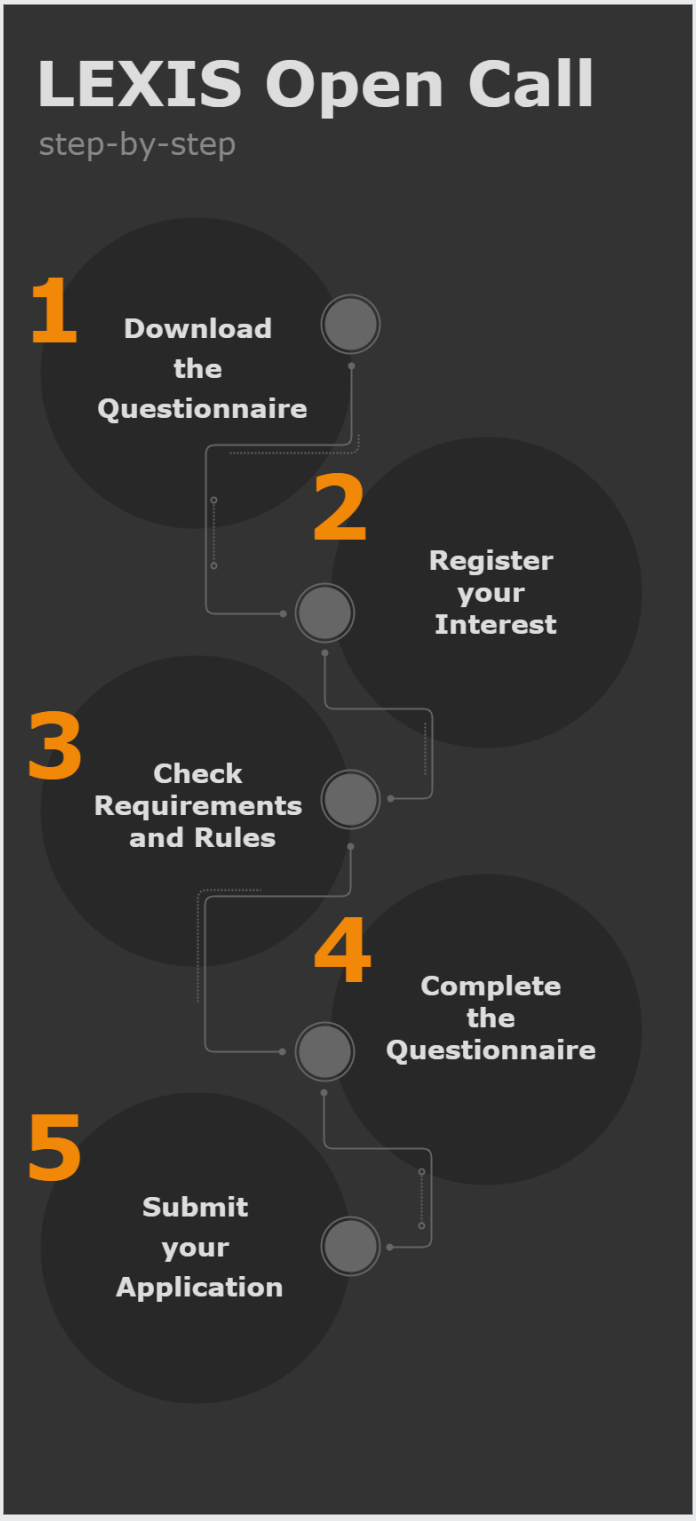
5. Submit your application using your login information. You will be notified via e-mail about the status of your submission.

Every candidature will be presented once a month to the Selection Committee until June 2021.

The Open Call will stop recruiting new application experiments/projects when the computing resources (CPU/GPU/FPGAs – millions core hours) are fully allocated and/or at the **end of June 2021.**

The selected application experiments can run on the LEXIS infrastructure up to the **end of November 2021** (depending on the COVID-19 situation, these deadlines might be extended).

We are proud to announce that multiple projects from all over Europe have already been selected and involved under the LEXIS Open Call initiative, covering various application domains (engineering, drug discovery, weather & climate, COVID-19).



LEXIS OPEN CALL

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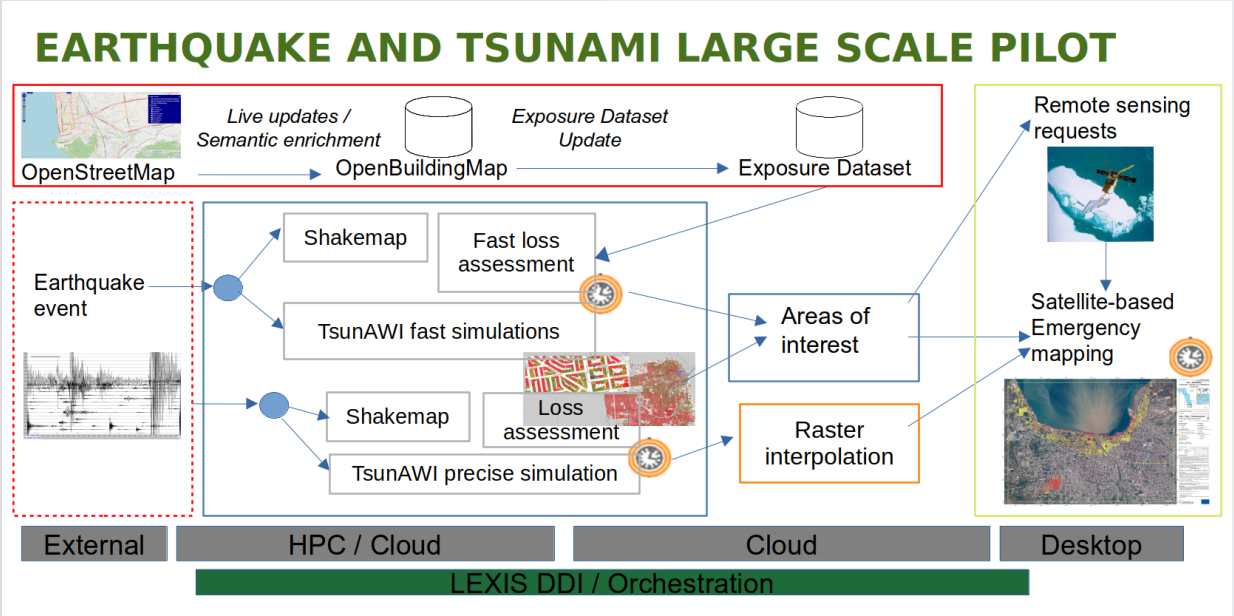
The Earthquake and Tsunami Large-Scale Pilot presents its Workflow

In the LEXIS project, one of the objectives is to demonstrate running complex simulations under real-time deadlines in order to get predictions in time for decision making and disaster mitigation.

In the **earthquake and tsunami large-scale pilot** of the project, tsunami inundation simulations and earthquake loss assessment are combined in a workflow, triggered by earthquake events. This pilot has progressed well, and its technology is now presented and shared, especially to support the LEXIS Open Call initiative. Some of the results were also featured during the "HPC for Urgent Computing" workshop at SC20, showing that the broader topic is of common interest for the HPC community.



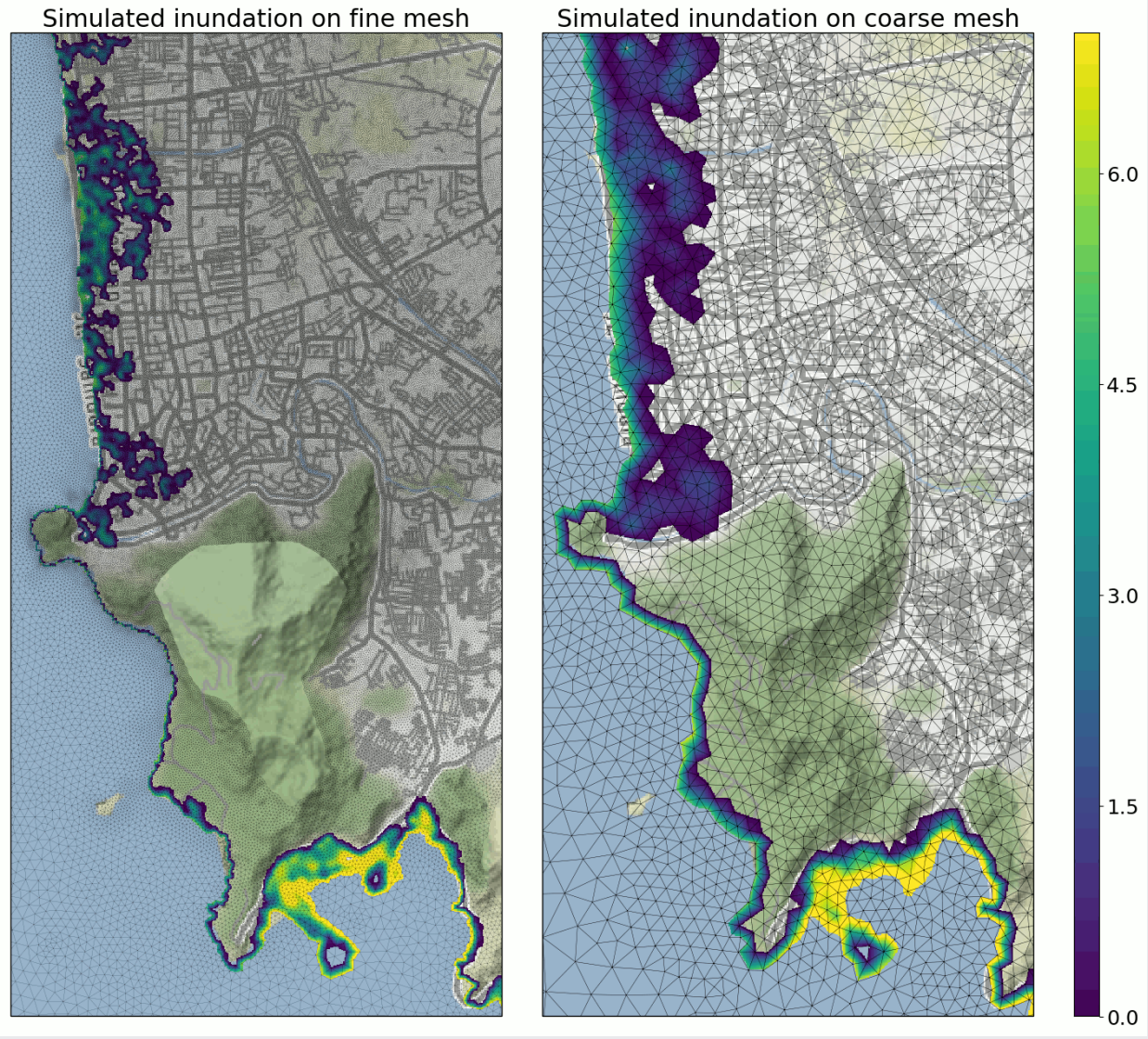
The earthquake and tsunami workflow in LEXIS

How does the earthquake and tsunami workflow, shown in the previous figure, work?

First, we need an up-to-date inventory of potential victims and damaged structures, which is provided by a 24/7 data flow around the OpenBuildingMap system. It is updated out of OpenStreetMap data. The “Exposure Dataset”, within a fast, optimized database structure, then provides condensed information on the vulnerability of buildings around the world, including the people in those buildings.

The second element in the pilot is the event-triggered part. It is triggered when an earthquake happens, and has two branches: a fast path, and a precise path.

The fast path is triggered with the early earthquake event information, which initially is only the hypocentre: the earthquake starting location, depth and magnitude. When such an event occurs, it starts a LEXIS workflow that computes a shakemap, fast tsunami simulations with TsunAWI, and a fast (aggregate) loss assessment from the exposure dataset. TsunAWI optimisations have allowed us to calculate **inundation predictions on a coarse mesh** of the area (see figure) sixty times faster than with our detailed simulations (executed then in the precise path), reaching as little as five seconds of runtime.



Inundation maps for both a precise and a coarse mesh. The faster coarser calculation already provides valuable information.

The precise path is triggered a few minutes afterwards, upon the reception of the earthquake moment tensor information. This activates another, more precise shakemap generation, a detailed loss assessment, and a precise tsunami **inundation simulation on a finer mesh** (see figure). And again, the jobs are triggered via the LEXIS orchestration tools.

The final part of this workflow is a satellite-based emergency mapping process, where remote sensing images are analyzed to produce fast damage assessment maps for affected areas (Izmir in Turkey is a recent example). A core component here is the procedure for the quick identification of potential areas of interest by crossing event related datasets (i.e. shakemaps and inundation maps) with exposed assets, prioritizing them based on the potential impact. The fast identification of those areas based on objective criteria allows a more aware and solid satellite image acquisition process.

One of the key elements of the workflow is that interfaces are standardized and would allow for possible replacements of components and the inclusion of additional information. The core workflow infrastructure is designed to intrude as little as possible into the working of individual elements of the flow. For example, more tsunami simulations could be added, providing inundation maps to the areas of interest determination procedures. Additional shakemaps could be generated by seismic simulations. All such additions render the workflow more resilient against possible failures of individual predictions, and are ideally included in the framework of LEXIS Open Call collaborations.

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Ystia/Yorc LEXIS Orchestration Toolkit

This article provides the highlights about the orchestration technology, which is used in the LEXIS project to manage complex scientific application workloads.

The LEXIS execution platform tightly couples and federates multiple heterogeneous resources to facilitate workflows mixing HPC, IaaS-Cloud and Big Data (BD) requirements. Resource federation is a key aspect for successfully supporting current and future workloads e.g. in the AI sector.

At the basis of the LEXIS platform, the LEXIS Orchestration Service is built on a flexible orchestration solution (Ystia) developed by Atos, which combines a front-end system (Alien4Cloud) and an orchestration engine (Yorc).

Alien4Cloud allows to model applications using the TOSCA format, while **Yorc** provides large flexibility in controlling Cloud and HPC resources. Both have been extended to manage the deployment and execution of workflows across geographically distributed HPC and Cloud resources. Tasks such as simulation, data management, and remote visualization of processed data can be orchestrated, and Urgent Computing constraints such as those of the Earthquake and Tsunami Pilot can be met.

Additional capability, the dynamic selection of the most suitable resources for running different tasks composing a workflow, is also included. Relying on a monitoring infrastructure, the LEXIS Orchestration Service will be able to select these resources based on the best tradeoff of multiple selection criteria, while also allowing for the mitigation of consequences of site failures due to events like unplanned maintenance, by a failover strategy.

In the context of LEXIS, the Yorc middleware will enable the following types of workflows:

- dynamic workflows,
- data aware workflows (managing data access),
- Urgent Computing workflows,
- job failover workflows.

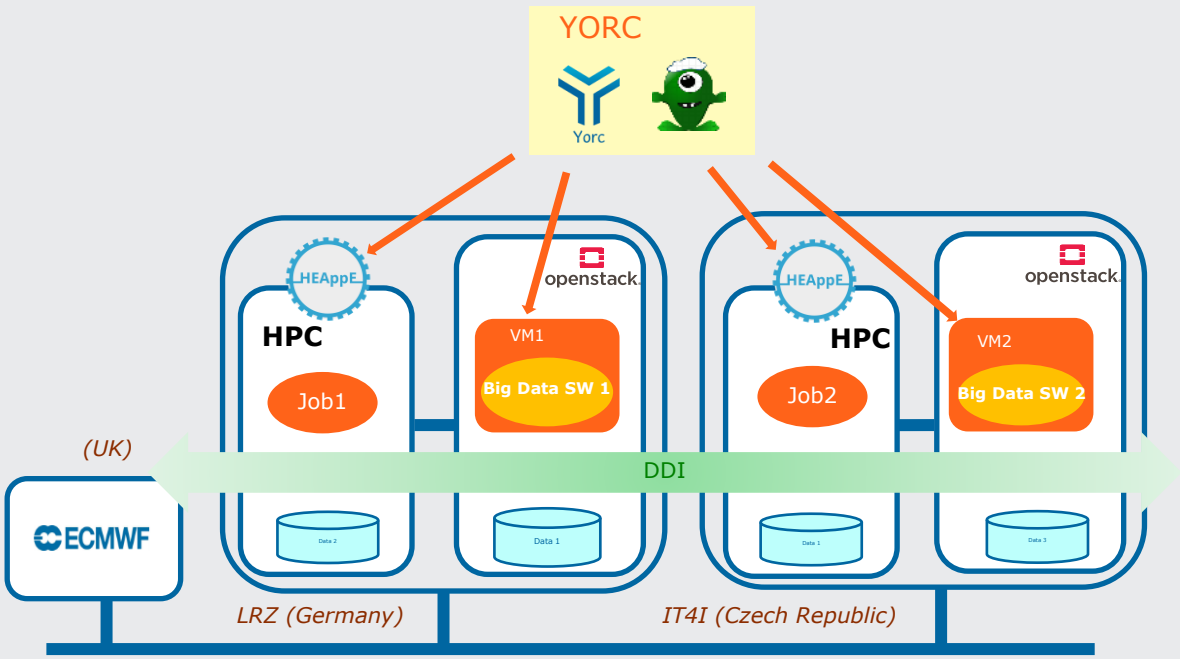
Yorc-based management of workflows

The figure below illustrates **how Yorc is used to manage workflows spanning the distributed infrastructures** in the LEXIS project, i.e. both Cloud (OpenStack) and HPC infrastructures at LRZ and IT4I. Yorc is able to orchestrate HPC jobs through any HPC schedulers, like SLURM, or PBS using **HEAppE**[1] as the middleware.

In this context, HEAppE, IT4Innovation´s HPC-as-a-Service framework, facilitates unified access to all LEXIS HPC systems for executing jobs or obtaining data.

Yorc also performs Cloud resource management e.g. the provisioning of OpenStack VMs in the example below. For the management of shared data during workflow execution, Yorc makes use of the LEXIS Distributed Data Infrastructure (DDI).

The applications to be deployed are modeled using **the Topology and Orchestration Specification for Cloud Applications (TOSCA),** an OASIS consortium standard language to describe an application made of components, with their relationships, requirements, capabilities, and operations. The Yorc front-end, Alien4Cloud, provides a studio for creating applications from an extensible catalog of TOSCA components, for deploying applications, and for running and monitoring the actual workflow instances.



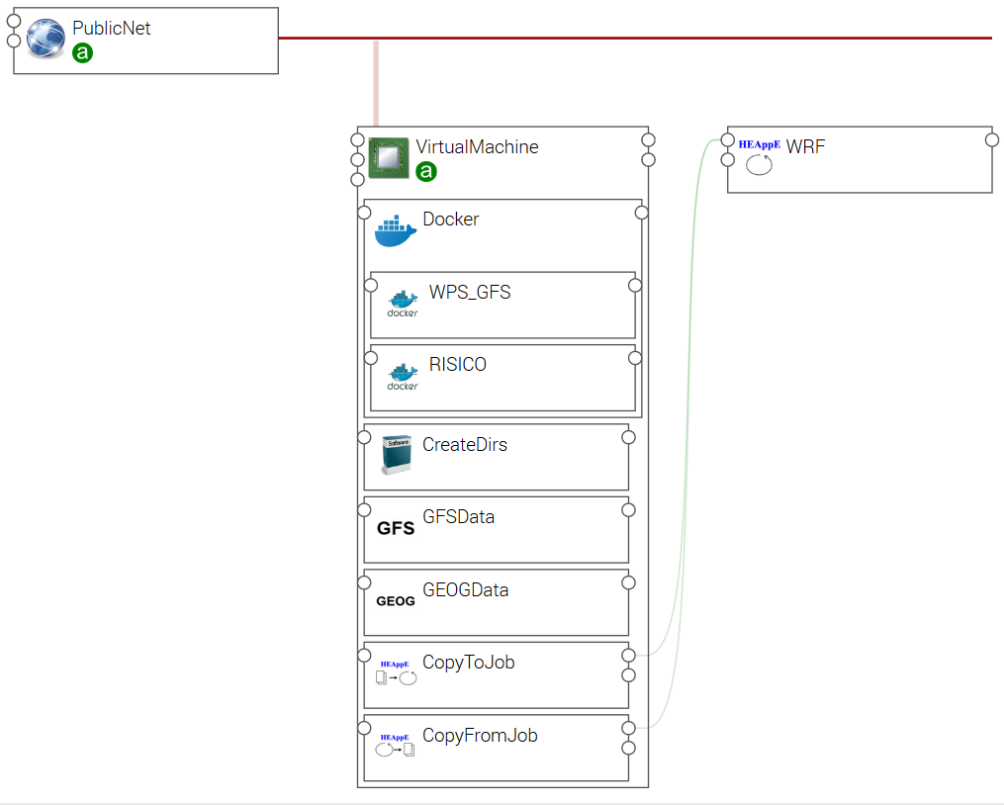
Application workflow execution over several locations with Yorc

[1]HEAppE middleware: http://heappe.eu – provides unified job management, monitoring and reporting, user authentication and authorization capabilities for HPC/data centers.

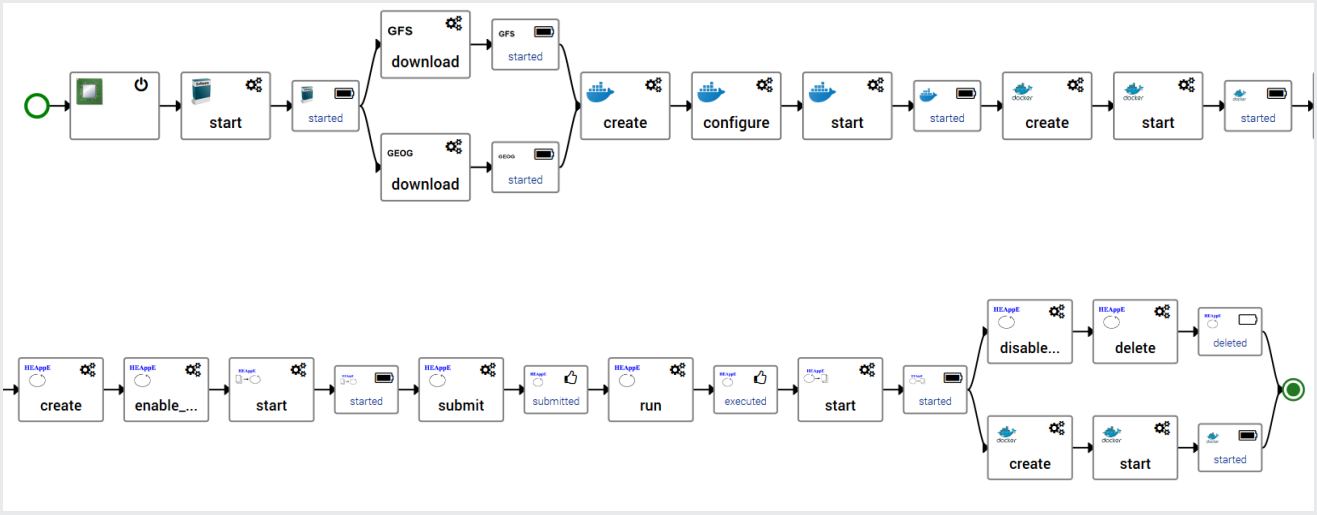
An example of a TOSCA application with its Alien4Cloud graphical representation is provided in the figure below. This TOSCA Application template represents a Virtual Machine that will be instantiated on a Cloud infrastructure, running some application components in Docker, and related through some data transfers to a job that will be launched on an HPC infrastructure.

The associated workflow in its Alien4Cloud graphical view is illustrated in the figure below**.**

This orchestration technology has been used in LEXIS to develop scientific workflows related to all LEXIS Pilots and Open Call use cases.



Graphic representation of a TOSCA application in Alien4Cloud



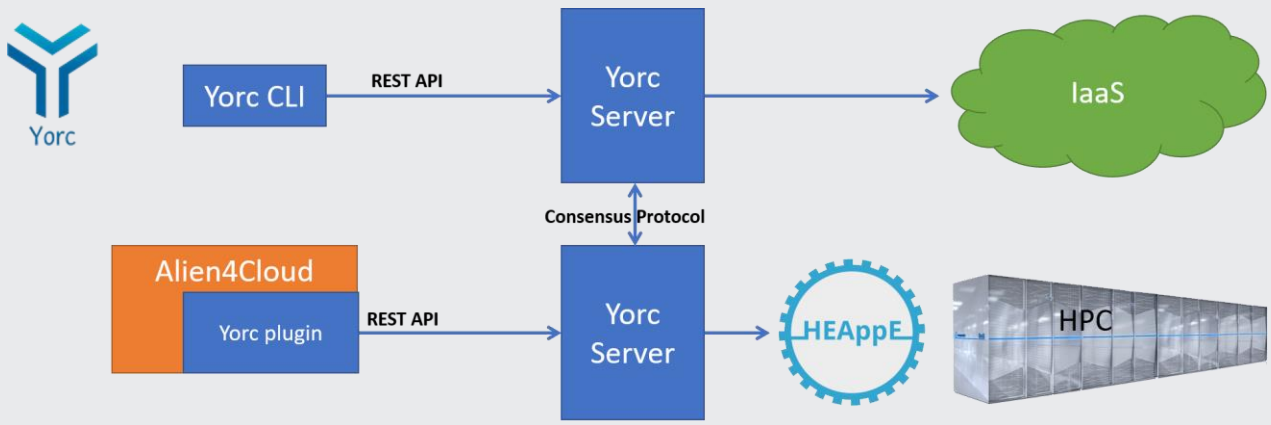
Workflow representation in Alien4Cloud

Yorc is based on a client-server and plugin architecture (see figure below). In the context of the LEXIS project, a plugin has been developed to support the HEAppE middleware, an intermediate framework used for handling job management, monitoring and reporting, user authentication and authorization over the HPC datacenters. It is also designed to use "placement policies" for dynamic resource allocation. Within LEXIS it will thus be connected to a "Business Logic module" developed by LINKS (LEXIS partner). This module uses monitoring and static system information to support the selection of the more suitable resources according to given criteria.

Further details on Yorc and Alien4Cloud techology

Yorc is a TOSCA native solution for complex applications lifecycle management and orchestration over hybrid infrastructures, open-source and available at https://ystia.github.io/. It is workflow driven and designed for large scale applications. It supports the whole application lifecycle (Deployment, Scalability, Monitoring, Upgrade, Recovery), exposes a REST API, provides a Command Line Interface (CLI), and can be used through Alien4Cloud.

Yorc supports many kinds of infrastructure (Google Cloud Platform, AWS, OpenStack, Kubernetes, SLURM HPC scheduler, HEAppE HPC meta scheduler) and various implementation artefacts for the TOSCA components (Bash, Python, Ansible).



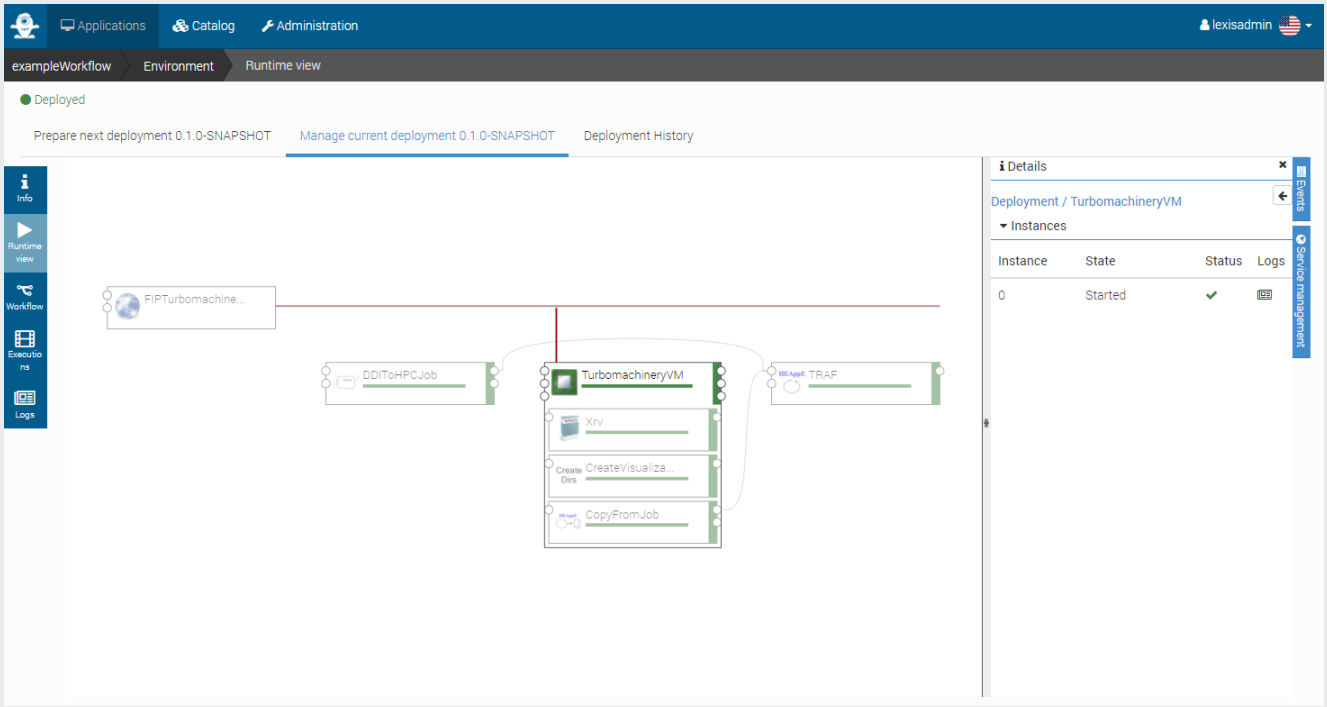
Yorc High Level Architecture

Alien4Cloud is the front end for convenient development of workflows for Yorc (see figure below).

It provides:

- a TOSCA component catalog which allows to register, version, and share TOSCA types,
- a TOSCA topology designer which lets you compose applications based on components from the catalog, and to instantiate a portable application, and
- a runtime control tower to monitor runtime deployments.

Based on TOSCA extensions, Yorc provides capabilities to manage HPC jobs and containers in LEXIS. It is developed in Go language. Although being available in Open Source, it is part of a larger Atos product, Atos CODEX AI Suite, providing both the Yorc orchestration solution for hybrid deployments, and a Machine Learning toolbox (FastML). This toolbox relies on Yorc for handling Machine Learning trainings deployment on HPC infrastructures.



Alien4Cloud Application Management Screenshot (runtime view)

LEXIS
Activities in brief

JANUARY 2021

101st AMS (American Meteorological Society) Annual Meeting,
January 10–15, 2021 , digital

- **Paola Mazzoglio (ITHACA)** presented a poster entitled **"Heavy Rainfall Identification within the Framework of the LEXIS Project: the Italian Case Study"** that highlights high resolution forecasts from the WRF-ERDS workflow (Weather Research and Forecasting - Extreme Rainfall Detection System workflow, developed by CIMA and ITHACA). An operational early warning system with significantly improved capabilities, running on LEXIS Cloud/HPC ressources, is the result. **Poster:** https://bit.ly/3bbjOeu

HiPEAC 2021,
January 18–20, 2021, digital

- **Jan Martinovič (LEXIS project coordinator, IT4I)** and **Alberto Scionti (LINKS)** attended the 4th **"HeLP-DC: Heterogeneous and Low Power Data Center technologies" workshop** (part of HiPEAC 2021), presenting an overview of LEXIS progress and key results. The workshop was organized around European funded projects belonging to the H2020 (LEXIS, EVOLVE, CYBELE and DEEPHEALTH) programme with the contribution of the Heterogeneity Alliance (HA) and industry representatives. It fosters the sharing of results, lessons learned, ideas, technological solutions and visions on Exascale HPC and the convergence with AI, Cloud Computing and Big Data. **Workshop:** https://bit.ly/2NBY5UZ

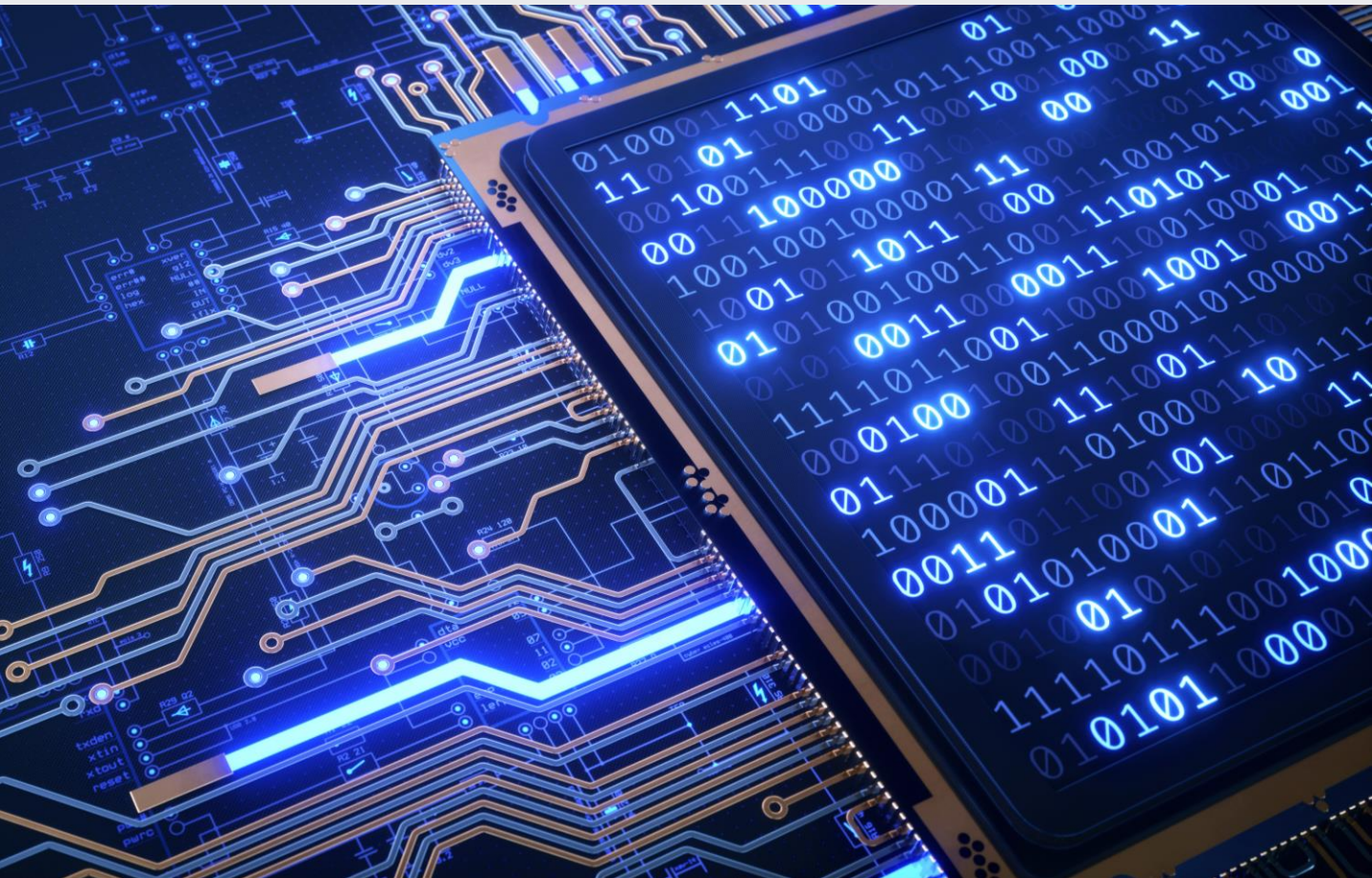
Tech forum “CFD TRAF code GPU porting: needs, results and applicability”,
January 26, 2021, organized by **Avio Aero**, digital

- **Ennio Spano (Avio Aero)** laid out more than two past years of continuous improvement in the TRAF code and its porting to GPUs, a work in collaboration with the University of Florence and IT4I/LRZ HPC teams. Problems faced and results achieved were highlighted, as well as development plans for 2021. The audience highly appreciated the efforts of the entire LEXIS team.

FEBRUARY 2021

Webinar on “LEXIS Open Call: How to apply to be a tester of the platform?”,
February 23, 2021, digital

- In collaboration with Torino Wireless Foundation, **LEXIS partners TESEO and LINKS** have organised a webinar reaching out to HPC, Big Data and Cloud enthusiasts from industry and SMEs, to inform them about the opportunity to test their workflows on the LEXIS platform. The event covers the Open Call processes from registration to candidate selection, as well as the implementation phase.



MARCH 2021

Workshop on High Performance Computing & Applications, organised by ODTÜ METU, March 6, 2021, digital

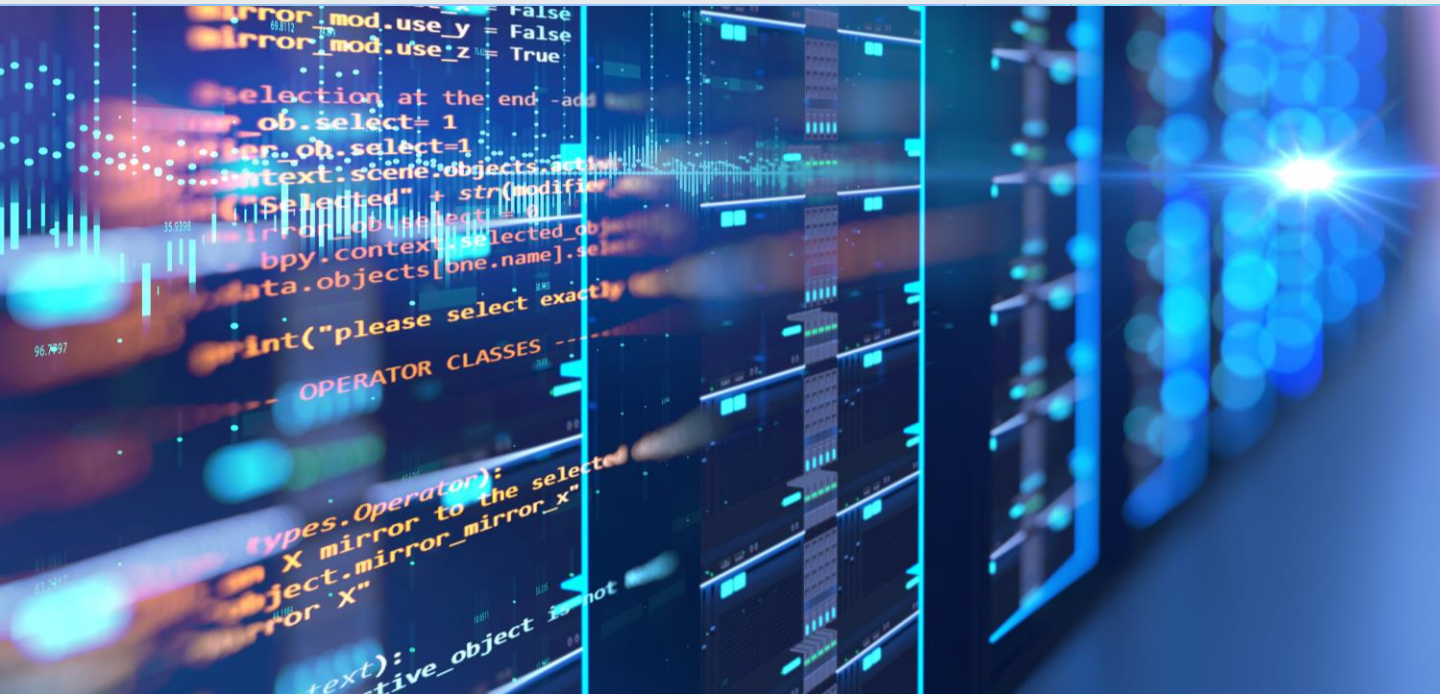
- **Jan Martinovič (IT4I)** gave a presentation **"The LEXIS platform for advanced computing and Big Data"**. In the talk, the platform architecture was described, highlighting the used technologies.
  Workshop: https://hpca.toplanti.info.tr

The International Symposium on Grids and Clouds (ISGC) 2021, organised by ASGC, Taipei, March 21–26, 2021, digital

We cordially invite you to follow the broad and exciting overview of the LEXIS project at this conference, for which you can sign up for free.
Event:
https://indico4.twgrid.org/indico/event/14/

- **Stephan Hachinger (LRZ)** gave a presentation **"HPC – Cloud – Big Data Convergent Architectures and Research Data Management: The LEXIS Approach"** in the "Converging High Performance infrastructures: Supercomputers, Clouds, accelerators Session I" at 15:00–16:30 CET on March 25, 2021

- **Thierry Goubier (CEA)** and **Antonio Parodi (CIMA)** showcased **results of the "Earthquake and Tsunami"** and **"Weather and Climate"** Large-Scale Pilots at the **"Deeper Understanding of Natural Disasters: Joint DMCC, UND and Environmental Computing Workshop"** within ISGC 2021 on March 24–26, 2021.



EuroHPC Summit Week 2021 / PRACEdays21,

March 22–26, 2021, digital

This excellent event gathers technology suppliers, HPC infrastructures, scientific and industrial HPC users in Europe.
Event: https://events.prace-ri.eu/event/1018/

- **Jan Martinovič (IT4I)** represented the LEXIS project at the **HPC, Big Data, IoT and AI future industry-driven collaborative strategic topics workshop**, organised by BDVA/DAIRO. **Workshop:** https://bit.ly/3ffa3iP

- **Thierry Goubier (CEA)** also represented LEXIS at **the European Urgent Computing Workshop** panel on HPC Urgent Computing. **Workhop:** https://bit.ly/3kGIC28

- **Donato Magarielli (Avio Aero)** gave a talk on **"Aeronautics Large-Scale Pilot in the EU-funded LEXIS project: context, objectives and first outcomes" at PRACEdays21 Industry Track.** His talk highlighted initial outcomes and results from evaluating the industrial applicability of the current-generation HPC/Cloud/BD platform built within LEXIS, through two case studies i.e. turbomachinery and rotating parts.

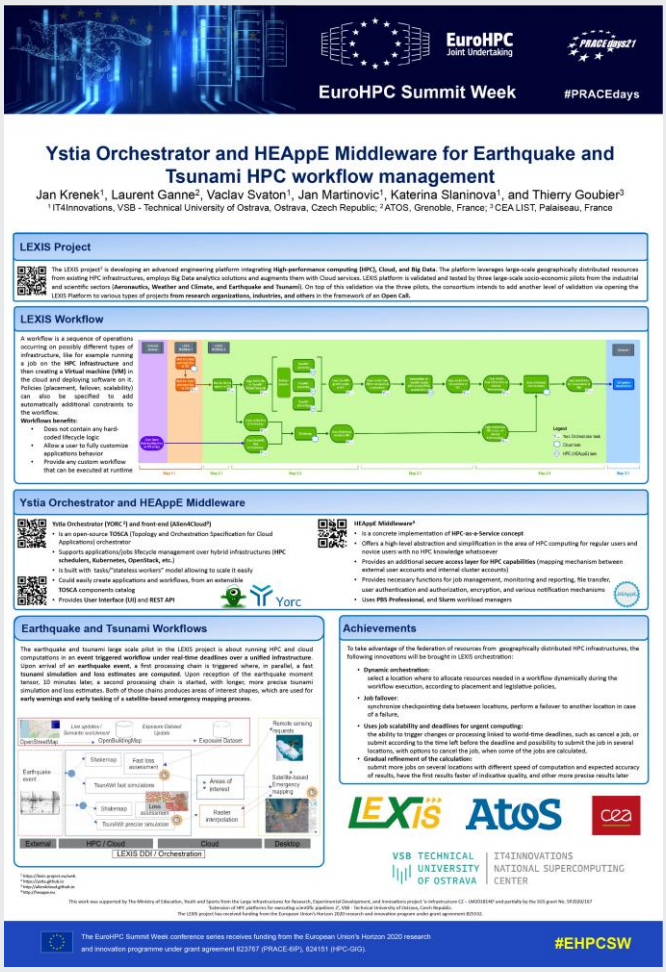
- **Jan Křenek (IT4I)** represented the IT4Innovations National Supercomputing Center and LEXIS with the **poster "Ystia Orchestrator and HEAppE Middleware for Earthquake and Tsunami HPC workflow management".** The poster expands on some exciting topics touched on in this newsletter.

APRIL 2021

EGU General Assembly 2021 – vEGU21,

April 19–30 2021, digital

- We congratulate **Natalja Rakowsky et al. for their work on "Prospects of real time tsunami inundation estimates with TsunAWI - Studies in the LEXIS project"**, which is scheduled as the vPICO presentation at the vEGU21.
  Session: https://bit.ly/2Or7bnE



This work was supported by the LEXIS project funded by the EU's Horizon 2020 research and innovation programme (2014-2020) under grant agreement No 825532