# Content

Galileo Conference

Consensual Document

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Autorship
Contributions

All the attendees to the 11th EGU Galileo conference (see Appendix) participated in the conceptualisation of this document during the breakout sessions and subsequent plenary discussions.

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Executive Summary

The 11th Galileo Conference of the European Geosciences Union (EGU) focussed on “Solid Earth and Geohazards in the Exascale Era”. This consensual document contains the main outcomes and conclusions from the conference breakout sessions, in which participants openly shared their knowledge and experiences to blueprint roadmap recommendations.

• At the European level, an ecosystem of synergistic projects is boosting the role of HPC in Solid Earth although difficulties exist in terms of recruitment of new specialized personnel and lack of transversal cross-domain software technology components. Best practices from software engineering are being progressively assimilated and adopted by our community although, beyond the ecosystem of Centers of Excellence (CoEs), few effective mechanisms exist for computer scientists to deeply collaborate with Solid Earth domain-specific scientists.

• Many Solid Earth codes are ported to accelerators but the variety of hardware architectures and programming models requires a major investment on portability software layers in order to follow the quickly-evolving vendor-driven heterogeneous hardware path.

• Solid Earth use cases rely on workflows with different levels of sophistication and complexity. Programming models like PyCOMPSs are being adopted for easier development and deployment of applications in distributed infrastructures. There is a clear need for higher workflow modularisation in order to improve and interoperate smaller tasks (building blocks, microservices) without decreasing the overall capability of the whole system.

• Training in HPC at all career stages is very necessary to bridge the gap between computer scientists and natural sciences. EuroHPC could consider enabling a unified training access mode, particularly on their GPU-based systems. This could, perhaps, be pioneered by the pan-European EUMaster4HPC and be extended also to CoEs, National Competence Centers (NCCs), and academia through periodic calls.

• The EuroHPC access modes are well-known and used, but current accessibility could improve through a unique authentication in a federated system of European machines. On the other hand, many of our workflows involve real-time data streams, and the automation of data transferring and the overall workflow executions are often hampered by system security reasons (e.g. double authentication with tokens). This is particularly critical in the
case of urgent computing because the intrinsic time-to-solution constraints of these problems require a high degree of automation on a 24/7 basis.

- The readiness level of several urgent computing services for natural catastrophes is high. As a community, we should articulate and lead a sound proposition to the EuroHPC JU (involving also the rest of agents concerned) in order to set the agreements and protocols for an effective urgent computing mode.
1. Introduction

The Galileo conferences of the European Geosciences Union (EGU) are small-scale and informal events to promote in-depth discussion among experts on cutting edge topics at the frontiers of geoscience research.

The 11th Galileo Conference (Barcelona, 23-26 May 2023), endorsed by the Center of Excellence for Exascale in Solid Earth (ChEESE), focussed on “Solid Earth and Geohazards in the Exascale Era”. The conference gathered 78 participants from 15 different countries, to address both the challenges and opportunities that Exascale computing presents for geosciences.

Most attendees came from European-based research institutes and academia, although other institutions worldwide were also represented by individuals (e.g. from the USA, China, and Latin America). Despite the European scope and focus of the meeting, these external contributions were very much appreciated.

The conference was articulated around 4 sessions linked to corresponding trending topics: preparation and optimization of High Performance Computing (HPC) applications (Session 1), edge-to-end data workflows (Session 2), state-of-the-art in computational geosciences (Session 3), and research infrastructures and EuroHPC access modes and policies (Session 4).

Each session was motivated by a keynote presentation followed by a series of invited talks and poster sessions. In addition, all sessions included breakout sessions in which participants were randomly divided into smaller groups to enhance debate and discussion on session-related key questions.

Moreover, the Conference also included a series of pre-meeting Master Classes in which 22 Early Career Scientists (ECS) were trained and mentored, of which 10 received financial support from EGU.
This consensual document reflects the main outcomes and conclusions from the breakout sessions, in which participants openly shared their knowledge and experiences to blueprint roadmap recommendations.

It is clear that a reduced number of individuals cannot speak on behalf of the vast community of the (European) computational Solid Earth scientists. However, we consider that the group of attendants was large and diverse enough to represent the different opinions existing in our community and to include the views on how challenges posed by Exascale computing may be addressed.
2. 
Topics discussed during the Conference

2.1 Current status of computational Solid Earth

*Sensu stricto*, the term Solid Earth refers to the Earth’s interior and its solid surface. However, the term is often used *sensu lato* to include phenomena triggered within the Solid Earth domain but that propagate through, and interact with, other geospheres, e.g. tsunamis, volcanic dispersals in the atmosphere, sediment transport, etc. Considering this broader definition, it was noted that the use of HPC across the different Solid Earth disciplines remains very heterogeneous. For example, surface and subsurface hydrology or sediment transport (including landslides) are not broadly addressed within the HPC world, whereas scalable applications to model geothermal energy systems, energy storage, or underground waste disposal are still poorly represented except for a limited number of remarkable initiatives (e.g. the GEOS, MOOSE, PorePy, or OpenGeoSys codes). Another untapped aspect is the interaction with the biosphere or even among different disciplines within Solid Earth geoscience.

The diversity of Solid Earth applications and their level of HPC-readiness is very broad. While some communities (e.g. computational seismology) are heavy HPC consumers and have been developing highly-scalable software for many years, other communities are just starting on this path. Codes may exist, but often with legacy issues and written by application scientists, such that it is critical to refactor them in collaboration with computational scientists and software engineers.

At the European level, several synergistic projects are boosting the role of HPC in Solid Earth, with substantial funding secured up to 2026. The first phase of the Center of Excellence for Exascale in Solid Earth (ChEESE-1P, 2018-2022, GA No 823844, 7.6M€, https://cheese-coe.eu/) was successful in leveraging other initiatives which built upon some of its developments. In particular, the Horizon Europe DT-GEO project (INFRA-TECH call, 2022-2025, GA No 101058129, 15.1M€, https://dtgeo.eu/) is developing a pre-operational prototype Digital Twin (DT) on geophysical extremes for future integration in the Destination Earth (DestinE) initiative, and the Geo-INQUIRE project (INFRA-SERV call, 2022-2025, GA No 101058518, 13.9M€, https://www.geo-inquire.eu/) will offer virtual and trans-national access to a set of Software as a Service (SaaS) and Workflows as a Service (WaaS) derived from ChEESE-1P (the so-called

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ChEESE-CoE Research Infrastructure). In parallel, the second phase of the Center of Excellence (CoE), now under the umbrella of the EuroHPC Joint Undertaking (2023-2026, GA No 101093038, 7.7M€, https://cheese2.eu/), is continuing the preparation of flagship applications in different Solid Earth domains (computational seismology, magnetohydrodynamics, tsunami modeling, volcanology, geodynamics, and glacier modeling) together with pilots and services on urgent computing, early warning, and hazard assessment. On the other hand, other initiatives beyond the Solid Earth domain are also playing a key supporting role to our community. Among these, the EuroHPC eFlows4HPC project (2021-2023, GA No 955558, 7.6M€, https://eflows4hpc.eu/), with one pillar fully devoted to solid earth hazards, is delivering a software stack for workflows and added-value HPC Workflow as a Service (HPCWaaS) platforms to facilitate the reusability of complex workflows in federated HPC infrastructures that directly fuel some of the DT-GEO and ChEESE-2P project developments. Another example is the already completed EOSC-synergy project (2019-2022, GA No 857647, 5.6M€, https://www.eosc-synergy.eu/), which implemented a Software Quality Assurance as a Service (SQAaaS) as well as FAIR data evaluators that are being adopted by (and integrated into) these other initiatives.

All in all, this ecosystem of aligned European projects is tackling Solid Earth applications, workflows, data analytics, AI and services, with emphasis on interoperability and data/software FAIRness, and embracing the three different ways our community approaches exascale computing (i.e., capability computing with “heroic” large-scale simulations, capacity computing with aggregated exascale workflows, and urgent computing). During the conference discussions, there was a general consensus on the remarkable attention that Solid Earth is receiving within the European HPC landscape, although some points of concern emerged regarding:

- Recruitment and appointment of new personnel. The aforementioned projects, intrinsically transversal and multidisciplinary, need personnel specialized in computational and computer sciences and in software engineering. In most countries, project partners are facing difficulties in hiring skilled colleagues because the public sector cannot compete with this labor market segment in terms of salaries and career expectations, adding to a gap in trained people for those truly R&D tasks. Several participants stressed that this hurdle can slow and, to some extent, hamper a timely implementation of the projects.

- Long-term funding sustainment. Although very substantial as a whole, this ecosystem of European projects results from aggregating a set of independent projects, each with different timings (3-4 years only), durations, and participants’ interests and roadmaps. In this sense, a comparison was made with the U.S. Department of Energy’s (DOE) Exascale Computing Project (ECP), a single sustained-in-time initiative to deliver domain-specific applications, software products, and other outcomes on the DOE supercomputing systems (Sierra, Summit, Frontier, and the upcoming El Capitan and Aurora exascale computers).

- Finally, it was noted that, similarly to the role played by the European Centers of Excellence (CoEs), the U.S. ECP has an application development pillar which also covers the Solid Earth domain (e.g. through the GEOSX project for multiphysics subsurface simulations or the EQSIM project for simulations of regional-
Many Solid Earth codes are already accelerated or being ported to Graphics Processing Units, or GPUs, e.g. under the umbrella of the ChEESE CoE or elsewhere. As in other disciplines, the variety of hardware architectures (e.g. AMD vs NVIDIA vs Intel GPUs) and programming models and runtimes (e.g. Kokkos/RAJA for performance portability). Unfortunately, this transversal component has no analogous counterpart in the European ecosystem of CoEs.

2.2 GPU programming models and paradigms

Many Solid Earth codes are already accelerated or being ported to Graphics Processing Units, or GPUs, e.g. under the umbrella of the ChEESE CoE or elsewhere. As in other disciplines, the variety of hardware architectures (e.g. AMD vs NVIDIA vs Intel GPUs) and programming models necessitates a major investment of time and effort in order to follow this quickly-evolving vendor-driven heterogeneous hardware path.

It was mentioned that, in some specific use-cases, GPUs are not used efficiently because: (i) the imposed workload (e.g. dictated by a given problem resolution) is too small to keep large throughput-oriented GPUs busy, (ii) the time-to-solution or memory problem constraints are strict, forcing to a strong-scaling solving approach (increasing the node count) that often results in the local (node level) problems being too small for GPU efficiency, (iii) a combination of the above. This may need code/algorithm rethinking and testing in order to run these cases of interest more efficiently on large parallel systems.

2.3 Software sustainability

Over the last years, code developers in our scientific community have started viewing software as an infrastructure, similar to hardware. Best practices from software engineering are being progressively assimilated and adopted by our community including, e.g., code styling, git-based repositories, CI/CD (Continuous Integration and Continuous Development/Deployment) pipelines, unit tests, benchmarking, automated documentation, etc. However, most numerical codes still rely on a very small number of developers (typically, less than five) which makes the continuous upgrade of the computational technology difficult. Scientists still need to better communicate and collaborate with computational scientists and software engineers and, although it was noted that this interaction is actually happening, some shortcomings were observed:

10.1 Interaction can be improved through the development of a common taxonomy and standardization of terminology and data (as recognised by initiatives like the open data standards).

10.2 Beyond the ecosystem of Centers of Excellence (CoEs), there are few effective mechanisms in place by which computer scientists can collaborate with domain-specific scientists to help on the development and maintenance of their codes. For many research groups, this lack of communication is costly and inefficient.

Sustainability of research software requires steady funding that in many cases comes somewhat discontinuously through short-lived projects (it was also recognised that flagship codes under the umbrella of CoEs are probably an exception). In this sense, the participants
encouraged the development of reusable and more modular codes, with components shareable across different applications and a shorter timespan from code prototype to production. Code sustainability is also linked to the readiness of researchers to collaborate on community codes and transversal community packages rather than focussing on single “hero” codes. Relying exclusively on large and complex community codes may hamper innovation, a hindrance that can be mitigated with younger codes, more flexible to adapt to technological changes and which may be designed from scratch for modularity, interoperability and sustainability.

2.4 Workflows

Computational scientific workflows can be defined as the execution of a series of interdependent tasks that typically involve data collection and preparation, data transfer, modeling, and analytics. Workflows are nowadays widely used in computational Solid Earth, although with different levels of sophistication and complexity. Similar to the case of code development, dedicated workflow management and orchestration systems developed by computer scientists are being progressively adopted by our community to, for instance: (i) run ensembles of calculations, (ii) perform concurrent execution of multiple communicating tasks on distributed infrastructures, (iii) propagate the FAIR data/software principles across the whole modeling chain (e.g. generation of new metadata associated with data processing, tracking of data provenance throughout the whole workflow) or, (iv) ensure portability and scalability across a variety of software and hardware environments (performance-portability). In particular, the conference showed several examples of the use of PyCOMPSs, an HPC-oriented task-based programming model increasingly used (not just in Solid Earth) for easier development and deployment of applications in distributed infrastructures.

13.1 On the possible uses of edge computing, the participants highlighted: (i) the capacity of triggering events directly near sensors (e.g. seismicity), (ii) the potential to on-site filtering large and yet useless volumes of raw data currently gathered (e.g. by fiber-optics networks), thereby reducing bandwidth needs during time-critical applications, (iii) edge computing could be used for community-driven information, harvesting information from multiple users in real time.

13.2 In terms of edge computing challenges it was noted that: (i) the connection with HPC is not straightforward, (ii) latency and interconnectivity can be an issue, (iii) at present we don’t really know/have the hardware required, (iv) resilience can be an issue because sensors themselves may fail at the moment of a disaster (power outages, accessibility problems) and, (v) challenges making the data actionable.
2.5 The growing role of data-driven modeling

The emerging and prominent role of Artificial Intelligence (AI) and that of Machine Learning (ML) and Deep Learning (DL) in particular was largely debated. Examples of data-driven simulations were presented for tsunamis, earthquakes, and glaciology, mostly in the context of urgent computing.

- On the AI/ML positive side (pros) it was stressed that: (i) Physics-Informed Neural Networks (PINNs) have been demonstrated to be very valuable in terms of decreasing time-to-solution, solving partial differential equations and inverse problems. PINNs are capable of combining both the representation learning and prior knowledge in the field, (ii) ML helps in combining real data with synthetic data (models can be trained with physics-based model datasets). DL models are trained to learn the representation of the desired output, this makes it suitable to bridge the gap between simulated and less represented real data during training, (iii) it is very useful in Uncertainty Quantification (UQ) studies and, (iv) it naturally scales very well.

- On the AI/ML limitations (cons) it was mentioned that: (i) ML strongly relies on the abundance, quality, and universality of data and/or simulation outputs, a limiting factor in our field, (ii) it cannot reproduce extrema if not present in the training datasets (we are often concerned with the tails of the event-probability distributions and datasets are normally depleted in less-frequent extreme events), (iii) it has poor extrapolation capabilities, (iv) in general, ML models still need to improve accuracy, need more scientific validation, and are not suited to all situations found in our domains, (v) it is heavily reliant on software packages developed by third parties and, (vi) the reluctance to embrace ML on the part of some scientists due to its black box nature (the underpinnings of the technology are not fully controlled, as opposed to numerical methods). This later aspect is also relevant to end-users and stakeholders. For example, it was mentioned that, in some cases, we have still not yet earned the full trust of some stakeholders with results we trust ourselves, and this will become even harder if our products/services rely on AI/ML approaches. In addition, some data-driven tools like ChatGPT have earned a negative public perception (media publish news on the dangers of AI), and this raised some concerns as to how data-driven early warning and forecast products may be perceived by the general public.

All in all, it was recognised that data-driven approaches have massive potential and should be invested in but, at the same time, we should not abandon support for purely physics-based modeling. AI/ML is not and cannot be everything: it is a tool (not the tool) and should be considered to be complementary to and coexistent with traditional approaches (both data-driven and physics-based modeling will have their spheres of applicability). In this scenario, our community may need expert assistance to fully understand the driving fundamentals, as we are supposed to explain and understand natural phenomena. ML/AI is, by nature, not great with regards to explainability.
In general, geoscientists have a limited background in computational sciences. Training in HPC as well as a basic knowledge of software engineering is necessary to have a more fluent communication with computer scientists. This actually concerns all career stages, from undergraduate to advanced senior researchers. The existing training activities (e.g. former PATC courses, domain-oriented initiatives under the umbrella of CoEs) could be enlarged and extended also to under-graduate and pre-doctoral academic levels. A Masters Degree (MSc) could bridge the gap between computer scientists and natural sciences (children nowadays do coding in primary school, future academic courses could include more advanced coding on GPUs within their degrees).

The difficulty in accessing supercomputing systems for training purposes was noted (and actually reflected upon during the preceding Master Classes hands-on). For example, in many HPC-centers, security measures do not allow using a small part of their systems for training on GPUs; this adds artificial barriers for students and scientists to learn how to develop codes for such machines unless they are directly participating in certain projects.

EuroHPC could consider enabling a unified training access mode on their systems, allocating (and isolating) a small fraction of their tier-0/tier-1 infrastructures and make them available in a similar way as it is possible to access Microsoft Azure (or equivalents) for teaching purposes. This could, perhaps, be pioneered by the pan-European EUMaster4HPC and be extended also to CoEs, NCCs, and Academia through periodic calls in order to cover all the training levels and needs, from generic to domain-specific.

The current EuroHPC access modes (benchmark, development, regular, and extreme) were presented and discussed during the conference, which also debated:

- Benefits of a unique authentication for all European federated machines (similar to the FENIX infrastructure but at a tier-0 level). This could include the possibility of moving (sharing) a project from one system to another, making the optimisation and the architecture-ready deployment of applications more efficient. However, it was unclear how data transfer may work seamlessly in federated environments.

- In many of our workflows, particularly those involving real-time data streams, data transfer to (and retrieval from) HPC systems is hampered by volume and security restrictions. In some cases security penalizes productivity, and technical solutions to mitigate such an imbalance should be analyzed to deploy workflows more efficiently. The granularity of the safety levels in the U.S. systems (spanning from 1 to 5) was mentioned for comparison.

- There was a general agreement that we should lobby more actively for a real dedicated urgent computing (emergency) access mode in EuroHPC systems. The JU Governing Board No 18/2021 stated that “the JU Governing Board may grant a small percentage of access time without a call for expression of interest in some exceptional cases such as strategic
2.8 Urgent and emergency computing

Urgent (super)computing in the context of natural catastrophes has been pursued for a long time within our community. Demonstrators and related services enabled at high Technology Readiness Level (TRL) have been developed in the context of the ChESE CoE and a few have even been used in real operational environments, e.g. during the 2021 La Palma eruption in the Canary Islands. Multiple aspects related to urgent computing topic were discussed during the conference, leading to some conclusions and recommendations:

• The identification of actors, stakeholders, and resources should be made on a case-by-case basis, depending on the specific hazard and affected region(s). To start, a few relevant cases (e.g. UC for earthquakes or tsunamis) could pioneer agreements and protocols between service providers (including institutions, problem specifications, codes and workflows involved, triggering conditions, etc.), data providers (including the ERICs), stakeholders (entities with legal mandates, regional or national-level emergency managers, civil protections, etc.), and HPC facilities.

• HPC centers will likely become reluctant to this access mode if perceived as disruptive for their regular operations. In this sense, unambiguous and official agreements need to be made on: (i) extent and specific purpose of the computational resources to be allocated, including robustness of the triggering mechanisms (triggering threshold based on event magnitude and risk exposure whenever available, while minimizing false alerts), (ii) technical solutions to minimize disruption of operations (e.g. a dedicated queue in which users know that jobs are “killable without warning” but that, for most of the time, can execute regularly under hibernated emergency-mode), (iii) redundancy of systems, ideally in a federated pan-European environment, as a way to palliate unavailable resources.

• At present, warnings and forecasts for geohazards exist in many operational centers at National Level, but in most cases without substantial (if any) HPC-based support. The deployment of urgent computing on different systems needs a taxonomy of the operational systems available, support for containerisation, continuous testing and exercising (to ensure readiness), and support to maintain all the underlying software stacks operational at all times and across several systems. This endeavor could mimic already existing infrastructures, e.g. the ECMWF-National weather centers-Copernicus, and responsible players must be identified for these purposes.

• The intrinsic time-to-solution constraints of urgent computing problems require a high degree of automation on a 24/7 basis. However, emergency management and...
decision making also involves many human-made decisions under uncertain and rapidly evolving scenarios that go far beyond HPC. In this sense, a traffic-light mechanism could be established for progressive (incremental) activation of emergency access mode resources. For example, if a triggering case occurs, HPC centers could automatically allocate a minimum pool of resources while an emergency panel makes a decision (to save time), but more resources could be added afterwards (hours or even days later) based on panel request(s).

- Stakeholders need to be involved at the earliest design stage, as requests must be triggered (and defined) by institutions with legal mandates at national or at European levels, e.g., the Emergency Response Coordination Centre (ERCC) of the EU Civil Protection Mechanism or the Aristotle initiative.

- Finally, on a scientific level, the need for better decision support systems (maybe AI based) both upstream and downstream of HPC workflows was highlighted, together with some challenges inherent to real-time simulation cases: (i) availability of data streams, (ii) limitations posed by bandwidth and latency, (iii) difficulties in full workflow automation and robustness, (iv) role of ML models in reducing time-to-solution and, simultaneously, their yet insufficient credibility of results, (v) workflows as the vehicle for interaction between data and simulations at near-real-time scales.

21 In view of all the above, it was suggested that, as a community, we should establish a group of discussion (task force) to articulate a sound proposition to the JU and the rest of leading agents involved. The agreements reached on the special access scheme with the DestinE initiative should be an inspiration.

2.9 Other aspects

22 To conclude, miscellaneous other aspects were also discussed:

22.1 Cascading and compound-hazard scenarios are poorly addressed. Our community needs to break down existing barriers to collaboration on different hazards in order to study better hazard interdependence and more complex processes, such as their interaction with the natural and built environment. Surely, new computational resources should facilitate this.

22.2 Better communication channels should be established to highlight the importance of our research to society (outreach, dissemination) and to support the decision-making process.

22.3 Finally, the potential applications of quantum computing in our field were considered in the decades to come, particularly on how hybrid quantum-classical computing can benefit ensemble-based modeling and uncertainty quantification. However, it was assumed that this discussion is still on a very vague and speculative level.
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The consensual document from the 11th EGU Galileo Conference gratefully acknowledges the financial support provided by the European Geosciences Union (EGU), the EuroHPC Center of Excellence for Exascale in Solid Earth (ChEESE) under Grant Agreement No 101093038 (https://cheese2.eu), the Ministry of Science and Innovation of Spain, the State Research Agency, and the European Union's Next Generation/PRTR Program through grant PCI2022-134973-2.