

Call for Proposals

Collaborations to prepare Europe's Weather and Climate Models for pre-exascale systems (ESiWACE3-S2-2024)

2024-2025

A joint call for proposals by the Netherlands eScience Center, Eviden, Barcelona Supercomputing Center and Swedish Meteorological and Hydrological Institute



Part of the Services provided by the ESiWACE3 Center of Excellence in Simulation of Weather and Climate in Europe

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1 Introduction

1.1 Background

Earth system models (ESMs) are typically large applications that are subject to ever-increasing complexity, intending to resolve an increasing number of physical processes and represent the Earth with higher fidelity. At the same time, there are significant investments to adapt the software to the latest hardware architectures. Generally, these improvements go hand in hand, as higher accuracy often can only be achieved through increased resolution or larger ensemble sizes, thus increasing the required computational resources. Where the model development is driven by scientific expertise, the performance optimization is driven by the desire to use computing resources efficiently and at a sufficient scale.

After a long period of relative stability, the computing infrastructure landscape is rapidly evolving and diversifying, with more change on the horizon. Adapting existing software to the latest computing platforms and exploiting the full capability of the architecture requires specific expertise in performance engineering, hardware accelerators, and programming models. As such, continued development of weather and climate models requires new collaborations between experts from different fields.

This call for proposals aims to support the scientific community in the adaptation of ESMs for the exascale-computing challenge: we create short collaboration projects, of a maximum length of 2 **person-months** (PMs), that provide engineering time, guidance, and knowledge transfer to help researchers in the adoption of tools developed in the framework of ESiWACE3 itself. All groups developing and maintaining ESM codes - not only the ESiWACE3 partners - can apply. Proposals will be subject to a review regarding technical feasibility by the service-providing partners (NLeSC, Eviden, SMHI, BSC) and undergo a review more focussed on scientific impact by an external committee. When found eligible, the project will be granted an in-kind contribution by one of these partners.

The **Netherlands eScience Center** is the Dutch national center of excellence for the development and application of research software to advance academic research. The eScience center employs a large team of eScience Research Engineers, who are experts in state-of-the-art computational methods and technologies and have a keen interest and experience in developing research software. The center harbors unique expertise in programming for heterogeneous hardware architectures, optimizing software for supercomputing platforms, and deploying technologies in the often extensive Fortran codes that govern the domain of atmospheric physics and oceanography.

The **Eviden** team in charge of the ESiWACE3 services, part of the Center for Excellence in Performance Programming (CEPP) team, is composed of experienced HPC experts involved in collaborative European projects in the weather and climate domain, but also in other domains. The core expertise of the team is HPC applications profiling and tuning on a variety of high-end HPC systems including heterogeneous systems, memory accelerators, etc. Thanks to Eviden's position as a European leader in HPC, the team has access to a wide set of state-of-the-art HPC hardware, software, tools, and knowledge.

The **Swedish Meteorological and Hydrological Institute (SMHI)** is leading the task "Support, training and integration of state-of-the-art community models and tools" which fosters improved user support, enhanced training, and faster integration of existing community models and tools, leading to enforced



user-driven evolution of the community software. Within this task they are responsible for the EC-Earth model, facilitating community-wide access, use of the model's latest versions, and diffusion of best practices.

The **Barcelona Supercomputing Center (BSC)** is a well-known leading supercomputer facility and software consultancy agency and host of MareNostrum, one of the most advanced supercomputers in the world. The BSC Earth Sciences department focuses on developing and implementing global and regional models and data solutions for air quality, climate predictions, and their applications. Its HPC team has unique knowledge of profiling and optimizing multi-component MPI applications, removing I/O bottlenecks, and accelerating algorithms using GPUs.

1.2 Purpose of this call

This call for proposals aims at supporting the ESM-developing communities in the adoption of tools, developed in the landscape of ESiWACE3, to help them improve the model efficiency and readying the software to enable model execution on existing and near-future (pre-)exascale computing platforms. A competitive proposal aims at having a long-lasting impact on (the main branch of) the source code of an established atmospheric or ocean model, or any other ESM component, to progress its capability of efficiently and effectively using modern computing hardware. To ensure such an impact, there is a strong preference for models developed under sustainable and re-usable software engineering practices and developed as open-source projects with a permissive open-source license.

Mixed precision: Kernel Tuner & AutoRPE

While mixed-precision techniques have spurred a lot of interest in recent years, with their promise of a substantial increase in throughput and reduction of the memory footprint, the difficulties that can be encountered in a "by hand" implementation have also made scientists skeptical regarding their adoption. To try to overcome this diffidence in the community HPC-experts have started developing tools for the automatic reduction of precision in ESMs. Proposals seeking support for this kind of solution can target two different tools, depending on the architecture supported: Kernel Tuner on GPU accelerators, and AutoRPE for CPU application. In both cases, the proposal should aim at reducing precision in the critical path of the code and tuning the resulting code for maximal throughput and/or higher energy efficiency on the chosen device. Scientific validation will be left to the applicant due to the reduced length of the service involved.

Cross-platform deployment: Spack and good practices

In the modern scenario scientists are more and more frequently required to deploy their code efficiently on different HPC platforms. This represents a real challenge, given the variety of architectures used, and the difference in the environments installed, on each and every one of the HPC machines available in Europe. The offered service targets those users seeking support to make their applications and their dependencies deployable and portable on different HPC systems, especially on EuroHPC JU ones. The successful applicants will receive help to use Spack, a package management tool designed to support multiple versions and configurations of software on a wide variety of platforms and environments on HPC clusters.



Furthermore, we can provide support to audit the applicant's build system identifying its flaws and ways of improvement. Good practices could be advised to improve portability, and maintainability and pave the way to support new hardware and software stacks (like different GPU technologies, different compiler stacks, different CPU technologies including ARM processors, etc.)

Apart from offering limited engineering time and implementing code modifications, the projects principally aim to provide guidance and establish knowledge transfer between HPC experts and modeling groups. We believe that code transformations can only have a lasting impact if the software maintainers have sufficient expertise in the technologies and techniques that are being used.

1.3 Available budget

In this call, each grant consists of in-kind support in the form of a team of skilled Research Software Engineers (RSEs) employed by either the Netherlands eScience Center, Eviden, SMHI, or BSC. The RSEs will work remotely on the project for **up to 2 person months**, to be spent over a period of **maximally six months** after the project starts. The hours will be planned flexibly and in mutual agreement with the applicant. Included in this time is the dissemination of the work, both internally in e.g. ESIWACE3 project meetings, and externally through conference and workshop presentations.

Given the total budget, up to three proposals can be granted as part of this call. After submission, the first round of grant decisions will be announced in **June 2024** and the applicants of awarded proposals will be contacted.

2 Guidelines for applicants

2.1 Who can apply?

This call addresses all European ESM developing groups, including atmospheric sciences, oceanography, and climate-related domains such as land or sea ice modeling, land-surface modeling, atmospheric or ocean (bio-)chemistry, etc. The call includes, but is not restricted to global models, and therefore regional models or small-scale very high-resolution applications such as atmospheric mesoscale models are eligible as well. Members of the ESiWACE3 consortium are allowed to apply for this call, but external groups have a strong preference. The applicant's institution needs to be located in one of the countries participating in the EuroHPC Joint Undertaking.

We aim to have a permanent impact on the source code of the application, and this is most likely achieved if the applicant is part of the core development team of the software; derived 'downstream' versions or user-specific branches will have a smaller chance of being granted, as we wish not to contribute to the fragmentation of the European ESM landscape.

2.2 What can be applied for?

The grant consists of **up to** 2 PMs of in-kind consultancy, engineering, and knowledge transfer time by one of the expert RSEs on high-performance and heterogeneous computing. These engineers will work remotely in small teams on the project and fulfill the hours within 6 months after the project starts. Each team will have a lead RSE who is the main contact point for the model developers. Throughout the service projects, the HPC experts are expected to work closely with the model development group to achieve ambitious goals in a short-lived project and establish the necessary transfer of knowledge to



ensure the maintainability of the developed code. Hence this requires active involvement from both sides. From the applicant, we therefore expect:

- Assigning (or being) a contact point from the model development group that actively participates in the development process and displaying an open, collaborative attitude towards the ESiWACE team; knowledge transfer can be pursued by reviewing code and organizing virtual pair-programming sessions.
- Guidance of the team of HPC experts by giving them access to the appropriate code repositories, providing representative test cases, describing validation procedures and coding standards, and helping them get access to specific hardware platforms (if requested in the proposal).
- •
- Filling in a short evaluation of the provided service after the hours are finished.

Since the work happens on a project basis, there is no available budget for long-term maintenance of the contributed code. The long-term maintenance will be the responsibility of the applicant's modeling group. The contributed code will be documented according to standard good practice, or the modeling group internal coding standards.

Finally, it is strongly encouraged that the applicant and the RSEs together promote and publish the work carried out in the project. These efforts are considered part of the collaboration, and the time for RSEs to spend on these activities is part of the in-kind budget of the grant.

2.3 When can applications be submitted?

This 'rolling' call is open from **March 4th**, **2024**, **14:00 CET** until **June 3rd**, **2024**, **14:00 CET**. After submission, a technical review is carried out by the service providers and a scientific review committee (Sec 3.1). Proposals submitted before **June 3rd**, **2024**, **14:00 CET** will be considered for funding starting in September 2024 and be fully reviewed by **August 9th**, **2024**. A second call will be open in March 2025 and closed in June 2025. Proposals granted in this second call will be considered for funding starting in September 2025. Note that the ESiWACE3 consortium reserves the right to update or change this call for proposals, including all key dates, after each review moment. Updated information on this second call will be published on the ESiWACE3 website soon.

2.4 Preparing an application

A proposal can be submitted by completing a Google form within the above time frame. The form consists of three sections addressing the following requested information:

- 1. A brief overview of the model, its scientific impact, and societal relevance. An explanation and underlying motivation of the deployment of the model at the exascale.
- 2. A brief description of the targeted platform or hardware architecture. The limiting factors to the large-scale deployment of the application onto the target platform and some ideas about what performance gains can be expected (the latter may be somewhat speculative).
- 3. Plans for the sustainability, dissemination, and maintenance of the developed software.

Applications must be completed in English.



2.5 Specific conditions

We expect the applicant to either provide or adopt basic infrastructure for remote software development such as a version control system, a platform to keep track of issues, progress, and discussions (e.g. Jira, GitHub, etc.), and to provide representative test cases for monitoring numerical results and performance of the program. In general, the applicant should display an open, collaborative mindset and is expected to give feedback to the RSEs during the development cycle. This means that the applicant is responsive to emails and announces periods of absence ahead of time.

The target hardware platform, together with all necessary compilers, firmware, and performance measurement tools, has to be available to the engineer during the development process. Access to the target platform can be established either through (i) a joint external (pilot) project call to a European facility, (ii) an internal EuroHPC allocation of the ESIWACE3 project, (iii) permission for some internal facility given by the applicant to the RSEs, or (iv) internal access of the RSEs to private or national supercomputing facilities. There is no guarantee from the service provider that the latter option exists or has a sufficient budget for benchmarking. In case the applicant arranges access for the RSEs, we expect sufficient resources (computing budget, disk space) and permissions to install the required tools.

If there are any visits of the RSEs to the applicant's institute, the applicant is responsible for providing the RSE with a suitable, safe, and healthy working environment. This includes providing an environment that is harassment-free and free of unwanted behavior, for more information see the <u>code of conduct</u>.

The applicant will write a short report to describe the progress that has been made by the collaboration, the impact on the performance or portability of the code, and the impact on the scientific use cases of the code. This report is due in March 2025 for projects started in September 2024. The specific format for this short report will be distributed in advance.

When the above conditions are systematically violated, the ESIWACE3 consortium may choose at any moment to stop the project funding. In particular, the first month of the project is considered to be a trial period, in which the effectiveness of the collaboration is evaluated and if deemed not effective the project can be terminated.

2.6 Submitting an application

The online application form will be made available on the ESiWACE website.



3 Assessment procedure

3.1 Procedure

First there will be a technical review of the proposal by one of the service providers. This review will not assess the scientific impact, but rather focus on the technical feasibility of the project: is the targeted performance improvement realistic, is the code practically portable to a new architecture within the timeline of the project, and can the underlying numerical algorithm be accelerated? We reserve the option to invite the applicant for a remote consultation meeting as part of the technical review process. The outcome of the technical review is binding, only a selection of applications will pass to the second round for scientific review.

The final decision on the grant will be made by an external scientific review committee of at least three renowned scientists in the fields of weather and climate, with an affinity for HPC. We will avoid reviewers who are direct colleagues of any of the applicants.

3.2 Admissibility and assessment criteria

A proposal is considered admissible if the applicant is affiliated with a European non-commercial research institution fulfills the description of 2.1, and there is no conflict of interest between the proposed project and the service providers. Furthermore, the code needs to have a license and the first-round reviewers (and eventual RSEs) need to be able to access the source code as part of the review process. Finally, the intended hardware platform has to exist within Europe, and obtaining access by the engineers to the hardware should be plausible.

The first round of technical review will focus on the following criteria:

- 1. Technical feasibility: are the proposed code changes doable within the 2 PM time frame? Is it plausible that the resulting code will run faster on the proposed target platform?
- 2. Technological state-of-the-art: are the applicants aware of the current state-of-the-art algorithms and techniques in their domain? Is the target hardware likely to be part of future European exascale machines and does the proposed work bring the application closer to exascale deployment?
- 3. Software sustainability and lateral impact: does the proposal provide a credible pathway towards sustainable software? Will the proposed changes be merged into the main branch of the model, and is this code sufficiently maintained by a community?

The second, decisive review round focuses on the scientific impact of the project, such as

- 1. Scientific quality: does the proposed work enhance the quality of the model output, does the increased performance of the model allow its users to reach unprecedented accuracy or enable scientific breakthroughs?
- 2. Scientific novelty: does the proposed work allow the model community to explore new territory, and use the software in other scientific applications?
- 3. Lateral impact: does the proposed work have a scientific impact in other areas or communities? Are there possibilities for generalization of the contributed software?



4 Contact details

4.1 Contact

If you have specific questions about this call for proposals and the assessment procedure, please contact:

Open calls at eScience center: Email: open-calls@esciencecenter.nl

For questions about the ESiWACE3 Centre of Excellence in Simulation of Weather and Climate in Europe, please contact:

ESiWACE3 Consortium Email: esiwace3-communication@bsc.es

For questions about the Netherlands eScience Center in the context of this call, please contact:

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6 Disclaimer

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