IS-ENES3 Deliverable D2.1

Infrastructure Strategy for Earth System Modelling for 2024-2033

What is needed to sustain large-scale European earth system modelling infrastructure from 2024 and beyond

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ABSTRACT

This document provides a set of recommendations which arise from an analysis of the European large-scale climate modelling needs carried out by the European Network for Earth System Modelling. There are detailed recommendations made under each of: HPC, Model Development, Collaboration, Diagnostics, Data Systems, and Workforce.

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Executive Summary

This document provides a set of recommendations which arise from an analysis of the European large-scale climate modelling needs carried out by the European Network for Earth System Modelling. There are detailed recommendations made under each of: HPC, Model Development, Collaboration, Diagnostics, Data Systems, and Workforce; this headline summary provides a summary of those recommendations.

I. For HPC, **the climate community retains a need for a range of classes of compute**: from institutional to world-class; from CPU to GPU; and from simulation focused to analysis focused. Such HPC will need to have sophisticated and performant storage systems and provide access to a wide range of users and user roles.

II. **There is a need for a more operational approach to some aspects of climate science**, but it must not be at the cost of existing or future research capacity; it is the research capacity which will ensure that the operational activity can be responsive to societal needs.

III. **The community should continue to invest in managing and sustaining shared infrastructure**. There are significant collaboration opportunities which require sustained funding and organised governance. Such collaboration comes naturally in scientific developments, but needs extra attention for technical developments.

IV. Model development (both scientific and technical) takes a long time, and is resource intensive. Significant work is still needed to improve raw simulation speed for all combinations of ensemble-size, complexity, duration and resolution. New algorithmic techniques are necessary. While increased collaboration is necessary, it should not be at the cost of unplanned reductions in model diversity. Whatever approaches are used to improve models and prepare for next generation systems, **modellers will need to pay more attention to the balance between the "three P's": performance (speed), portability (across platforms) and (scientific) productivity.**

V. **Large expensive modelling projects**, whether or not they are part of international collaborations, **need to be treated like satellite missions**: well publicised, and documented, engaging with user communities to support the maximum efficient use of data products, both ephemeral and persistent.

VI. **Shared diagnostic tools and libraries introduce efficiencies into the exploitation of model data**. The community should continue to seize opportunities to enhance sharing of such tools and continue to invest in the necessary underpinning libraries and conventions, all of which will need continual updating as new data formats, new methods of compression and new meshes are introduced.

VII. **Storage and data systems need to support a variety of use cases**, from analysing high volume data, to long term curation and sharing data into communities beyond climate science. Not all systems, software and formats will be suitable for all these use-cases; attention will need to be paid to how storage solutions meet the workflow requirements. Within that set of solutions, sophisticated cataloguing and distributed analytics will be important, as will be the ability to migrate data between storage tiers. Some data will be persisted for long periods, and shared between diverse communities, such data (and the simulation workflow that produced it) will need to be well documented and conform to FAIR guidelines.

1. Introduction

The European Network for Earth System modelling (ENES) was established in 2001 to "better integrate the European modelling effort with respect to human potential, hardware and software". In the intervening years the participants (institutions and individuals from across the European community and beyond) have worked together on a number of projects, including the previous phases of IS-ENES, the Infrastructure projects for ENES. IS-ENES1 led to the development of an infrastructure strategy for the ENES community 2012-2022[1]. The IS-ENES2 project updated it in 2017[2]. This document is the deliverable of IS-ENES3, and is the first public draft of the recommendations of a new version of that infrastructure strategy, fit for 2024 and beyond. The final version will be made public in summer 2023.

These recommendations arise from a strategic analysis of the needs of the European large-scale climate modelling community, which will be presented in "What lies beneath: a strategy for large scale European Earth System modelling from 2024 and beyond" Lawrence et al, (in preparation).

One important result from the analysis is that while many people and much computer capacity is deployed in modelling to service both understanding the climate system and projecting the future, the demand for products and services built on that modelling exceeds what can be delivered. In particular, there is a growing demand for the regular provision of reputable advice based on a new state-of-the-art predictive capability and expert interpretation. Such an "operational climate service" would need to harness pan-European expertise (including multiple different models), large and dedicated computers, and be supported by ongoing research. Such a division of labour is becoming prevalent in some countries, but a coordinated approach is necessary, albeit one that builds on, rather than replaces, existing activities. These recommendations do not address this need directly but provide a description of many of the characteristics it might have, and that are in any case necessary for the research community which would be needed to support such a capacity.

There are detailed recommendations made in two sections. The first addresses HPC and targets institutions providing high performance computing *for* the Earth system modelling community. The second section targets the earth system modelling community itself, with recommendations covering Model Development, Collaboration, Diagnostics, Data Systems, and Workforce. In the remainder of this introduction, we expand on the scope and mutual needs that have led to this joint

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[1] Mitchell, J., Budich, R., Joussaume, S., Lawrence, B., & Marotzke, J. **(2012).** *Infrastructure strategy for the European Earth system modelling community 2012–2022*. ENES Report Series 1. https://doi.org/10.5285/ca90b281d6ff4cffb9a9bbdeb5fa63f3

[2] Joussaume, Sylvie, Bryan Lawrence, & Francesca Guglielmo. **(2017).** *Update of the ENES infrastructure strategy 2012-2022*, ENES Report Series. https://portal.enes.org/community/about-enes/the-future-of-enes/ENES_strategy_update_2017.pdf

strategy. The document concludes with a review of the methodology that led to these recommendations.

The scope of the analysis covers the most intensive global Earth system and climate simulation, that is, simulation which requires major fractions of large machines over long periods of time, and/or the involvement of many partners across multiple institutes.

The main timescales of interest are decadal and longer, although of necessity, both process understanding and initialisation require the ability to look at shorter timescales. It is expressly not aiming to address the needs of Numerical Weather Prediction, although of course there are many overlaps in requirements and opportunities for synergy and collaboration. In the context of this strategy, we include as necessary infrastructure, all the necessary workflow to initialise, to run, to manage resubmission of checkpointed simulations, to manage and share the output data, and to do the analysis of those data.

The overarching scientific context is one of mutual dependency. No earth-system model is entirely "in-house"'; there are always dependencies on other components (technical and/or scientific) and other communities (often in other countries). We know that model uncertainty is an important part of our science, and so we know that multi-model ensembles and model intercomparison are important, and that these processes depend on shared data formats, vocabularies, and conventions. However, we recognise that everything we do requires more computational resources (with implications for cost and carbon dioxide emissions) and that building and maintaining our models is becoming ever more complex, taking longer, and involving more people. Few organisations have the necessary workforce to maintain and develop their codes, and large downstream communities are involved in data analysis, themselves utilising ever more complex analysis codes and piping climate model data into their own complex models.

Mutual dependency, and the dependency on third-party HPC infrastructure for large-machine access, leads to real difficulties with aligning effort efficiently, and makes co-design of projects and modelling systems within the science community and by the science community and HPC providers difficult, and sometimes, impossible. Major modelling codes can take a decade to fully develop and be in continuous evolution over a decade of production use – but hardware life cycles are much shorter, and codes may need to run on many different machines across the available provision. National funding cycles don't always align, and project overlaps can be short, and so requirements generated in one location may be difficult to meet using national funding elsewhere; the role of European Commission funding is crucial not only in its own right to facilitate common developments, but also in leveraging national funding and providing long-term continuity. It is also important that tools, data and modelling systems are well documented, allowing teams to pick up work done elsewhere when those third parties may not have the time and funding to provide either direct collaboration or support – this is particularly important for those simulation data products which target downstream communities, which may be in use for over a decade after their production.

2. Recommendations for providers of HPC computing to the climate community

2.1 Context

Computer architectures are changing rapidly, but Earth system modelling systems are changing much more slowly as they are very large complex codes with many interacting components. The individual components often have their own independent evolution, and where hardware changes might lead to the need for algorithmic changes (e.g. to provide the necessary arithmetic intensity to use GPUs efficiently), such changes may take many years to research and implement. In such cases this need for new algorithms means that this is not entirely a matter of "porting". As a consequence, many important climate codes and many important climate applications will not be accelerator ready (and/or efficient) within the next few years.

It is difficult to optimise model codes for performance, portability and (scientific) productivity (i.e., ease of manipulation by scientists). Climate codes can also be fragile with respect to both scientific and computational performance across major system and compiler upgrades.

Climate models result in large amounts of data which need to be analysed by multiple communities. The volume and velocity of such data is increasing to the point where managing, storing, and especially moving data for analysis is becoming problematic. The science community can only do so much to minimise the amount of such data, and so it will remain necessary to attempt to minimise data movement. Such minimisation can be best achieved by bringing analysis computation to the data, either in-flight (utilising data which may never reach persistent storage) or via data held on- or near-line for months to years. The individuals involved are likely to be working across institutional, national, and discipline/federation boundaries. The resulting workflows will be, unless there are federated user management systems, difficult to manage, insecure, and lead to users having credentials everywhere (with concomitant user management problems for HPC providers).

Not all data always needs to be accessible to parallel jobs with high bandwidth and low latency requirements. Many datasets may spend most of their time resident on tape (to reduce both financial and carbon costs), and much data when online may be best accessible via protocols which can be WAN or LAN (such as S3). Software support for workflow which migrates data between tiers will be necessary.

2.2 Recommendations

1. A dedicated European exascale facility would allow significant advances in climate science, but not all climate science requires exascale compute, and the necessary pipeline of model developments and improvements would rest on the continued provision of large national compute capabilities such as those provided in Germany via DKRZ and in the UK by the

Met Office. Hence, the climate community retains a need for a range of classes of compute, from institutional to world-class platforms with trans-national access.

2. National and International HPC providers should continue to provide large-scale CPU based HPC, alongside accelerated systems.
3. HPC providers should recognise the need to maintain compiler and operating system stability over long periods of service (major software upgrades can be as disruptive to science delivery as new machines). Where change is necessary, mitigation such as substantive periods with access to test and development systems should be provided.
4. National and International HPC providers should enhance provision for large-scale storage systems with co-located analysis compute, both CPU and GPU, suitable for machine learning and distributed analytic workflows.
5. Storage systems should include tiered storage which supports both high-performance data-analysis and the storage of exabytes of data, with minimal carbon cost and relatively (with respect to commercial) high turnover between tiers.
6. Systems providers should recognise the need to support a range of different access profiles for different users, ranging from full batch access to analysis compute access, storage only, and remote usage via gateway service software (e.g., DASK Gateway, WPS and other community standard protocols as they become prevalent).
7. Storage and analysis systems should have interfaces and user management systems that support membership of multiple different federations with differing authentication and authorisation regimes.

3. Recommendations for the climate community itself

3.1 Context

The major scientific theme common to all modelling groups is how best to address uncertainty in the context of global and regional change, including how that uncertainty is partitioned between the internal variability of the climate system, how knowledge of the climate system is implemented in models, and how we think humans may behave in the future. There are different and complementary approaches which stress different aspects of the importance of speed (and hence duration), complexity, ensemble size, and resolution to numerical experimentation. The major considerations for how to best use computing includes where and how to use higher resolution (everywhere or regional refinement?), whether processes can be emulated using machine learning, and how to balance the presumed increased fidelity of higher resolution models against the need for large ensembles to address variability and scenarios. Underpinning all these are technical questions around how to exploit parallelism, and what parts of which algorithms might be able to exploit mixed precision to increase speed.

Other questions revolve around how we can integrate other communities and modelling paradigms into the relevant workflows? Does the advent of causal network thinking which spans physical climate and other parts of the human and natural spheres lead to the need for different types of workflow and modelling? How can we make better use of observations, and can we say more about the future of important, but hitherto relatively neglected processes, such as melting land-ice?

These questions are reflected in major European projects addressing, amongst other goals, those of attempting to resolve storms (NextGEMS), to resolve the ocean mesoscale in centennial simulations (EERIE), to improve the representation of the full earth system response to anthropogenic emissions (ESM2025), and to extend the duration in time of ESM Simulations with a view to increased realism and an ability to further understand the interaction of climate change on a range of phenomena (OptimESM). Other projects are taking existing modelling systems but pushing them in some way to address important processes such as the Atlantic Overturning Circulation (EPOC) and the interaction of Oceans with ice (OCEAN-ICE). There are of course many other projects. Most projects, whether large or small, share an aspiration to address World Climate Research Programme (WCRP) goals and to prepare for future model intercomparison experiments. Current WCRP goals include delivering on their lighthouse projects – explaining and predicting climate change, safe landings for future climate, climate risk, and digital earths – and the European modelling ecosystem is gearing up for that work.

Together these activities lead to a spectrum of climate science which ranges from very long integrations of large ensembles of low-resolution models (e.g. ice sheet dynamics over millennia) through single model large ensemble experiments which utilise significant resources of both compute and storage (neither of which can utilise modern accelerated systems efficiently), to the highest-resolution global models which, although they are capable of fully utilising modern exascale systems, are limited in widespread applicability by speed, data volumes, and expense.

Maintaining all of performance, portability, and productivity is problematic with all these codes and requires significant effort, effort which is required even before the development of next generation codes can be entertained. The effort needed is growing in the face of expanding heterogeneity in computing.

The machine learning, data analysis, and other technical skills needed to exploit cloud computing and the massive parallelism inherent in modern HPC systems, are in considerable demand across all of science and society. Most groups are having difficulty recruiting and keeping sufficient technical expertise to both maintain existing capability and develop new capabilities, and this difficulty is exacerbated by the rapid pace of technical progress and growing needs to apply machine learning within both simulation codes and their analysis.

There is considerable scientific model diversity in Europe, and there is significant scientific benefit in maintaining that diversity, and even for some parts of the simulation realm, extending that diversity. That diversity extends across the codes themselves, with several major inter-related modelling families responsible for 30 different variant models which have contributed to the core experiments of the sixth phase of the coupled model comparison project (and which are responsible for over 40% of the simulated years contributed to that archive). Within that diversity, there is a common ocean platform NEMO used by many modelling systems, and soon a common sea ice platform (SI3); the community will need to be careful to reap the benefits of this common development without losing the benefits of diversity in modelling approach.

There is also considerable technical diversity in how the models are constructed. Recognition for the desirability of some shared development has resulted in a European coupler, OASIS, used by multiple groups for many years. Much of the community uses one of two common workflow systems (Autosubmit and Cylc), two groups are using YAXT for MPI communications, and recently the XIOS IO-server has been introduced into several models, but none of these tools are as widely used as OASIS. To what extent appropriate governance and development roadmaps can be put in place to allow more sharing of this technology is still a moot point, but there is little justification for many different technical solutions to the same technical problems (although there is also no justification for just one solution to each problem – there must be room for competitive evolution).

The complexity of analysis has led to the development of, and use of, many different analysis software systems. Most of the community exploit NetCDF for their primary storage, although copies of data held in Zarr are becoming more prevalent. Use of the Climate Forecast conventions remains crucial to sustaining interoperability of both commonly used tools such as xarray and the NetCDF operators as well as more targeted climate analysis tools such as Iris, cf-python, and the Climate Data Operators, CDO. Many groups have a standard simulation analysis package, such as the AutoAssess and CliMAF packages used in the UK and France. ESMValTool is also deployed at most sites, to provide a standard set of diagnostics which can be used to compare models and observations. Except for AutoAssess and CliMAF, all these tools are either used widely and/or are crucial to the maintenance of community standards, but even the local packages represent major investments in lowering the friction between simulation output and the delivery of scientific knowledge.

The most important community standard remains the Climate-Forecast conventions, and Europe has provided a considerable amount of the core effort sustaining these conventions over the last two decades. They support not only the interoperability of tools but are fundamental to the international community model intercomparison projects such as CORDEX and CMIP, which each have their own additional vocabulary and documentation profiles which need to be maintained and evolved. Europe has been a key leader in the development of tools (ES-DOC) for documenting numerical experiments and models in a way that facilitates both the execution of common experiments, and the intercomparison of model functionality – but these tools are currently nascent in capability and wide deployment, despite their obvious applicability in addressing both the propagation of institutional knowledge between communities and across time and space and in ensuring data products are FAIR: Findable, Accessible, Interoperable and Reusable.

Data systems have evolved from those which simply facilitated the bilateral sharing of subsets of data, to those which provided central archives of data shared from multiple groups, utilising the Earth System Grid Federation and publication protocols and technology that were originally developed for CMIP5 a decade ago. The data volumes associated with CMIP5, and particularly CMIP6 showed the benefit of centralised archives with co-located compute, and this model has become prevalent for major European collaborative model projects where partners are running large simulations locally and pooling simulation for analysis. However, as resolutions and ensemble size continue to increase new approaches are necessary, including the deployment of support for distributed analysis techniques (where for example a user workflow might include partial calculations carried out in several places with results pooled on the user's platform) – but it will remain important to enable centralised data analysis for the most complicated analyses. Nonetheless, it might not always be possible to centralise, or even save, all, or even any of, the highest resolution data products of a given simulation – leading to ``interesting'' feature subsets, and/or reduced resolution and/or reduced precision products, being the most widely shared. In such situations there will be an enhanced role for data analyses which make use of the high-resolution data "in-flight" (also known as "ephemeral" data). Such uses will include forcing third party models, cross-ensemble diagnosis, visualisation, and more – and many of the same issues around data standardisation will apply to the ephemeral data as the more widely shared production data.

3.2 Model Development

8. There is a need to sustain progress along the axes of ensemble size, complexity, and resolution, and this needs to be done without sacrificing duration requirements.
9. Not all modelling systems will need to advance along all axes, but there will be advantages in maintaining (European) model diversity in all directions.
10. The community would benefit from establishing what level of diversity is scientifically desirable and how best to organise itself to develop/sustain that level.
11. It will be important to seek out new methods to increase speed and decrease the cost of simulations. Key opportunities exist in the use of variable resolution, mixed precision, and machine learning, but it is also likely that completely new algorithmic paradigms will also be necessary.
12. Modelling systems will need to accommodate more flexibility in on-line diagnostics and interfaces with downstream applications.
13. Model output should use state-of-the-art compression techniques, and clearly document the impact of such compression on the inherent information content.

14. Model development practices should clearly identify their approaches to, and prioritisation around, each of performance, portability, and productivity.
15. With increasing complexity, larger ensembles and higher resolution, investments in complex internal technical infrastructure such as couplers and I/O servers will need to increase.
16. It will continue to be worth addressing impediments to sharing such infrastructures between groups; issues such as the need for shared roadmaps, shared governance, and documentation for non-local users.

3.3 Workflow

17. Large expensive modelling projects need to be treated like satellite missions: well publicised, and documented, engaging with user communities to support the maximum efficient use of data products, both ephemeral and persistent.
18. Workflow systems need to eventually develop common interfaces so third-party modellers can interface with more than one workflow system. Ideally these interfaces are consistent with data interoperability conventions and standards.

3.4 Collaboration

19. There is significant software in common across the community with concomitant international dependencies. Sustained governance and funding which recognizes differing funding horizons will be needed.
20. While not all modelling groups can develop, maintain, and evolve a full model system, there is still a need for model diversity which will reward groups which can contribute to important and/or unique model components.
21. Where experiments require large ensembles with independent simulations, opportunities for sharing the simulation load should be sought, particularly when they might involve adding additional model diversity and/or can exploit multiple HPC platforms. However, where ensembles are split in this way, care must be taken to carefully document the differences between any model variants as well as information about where the simulations were carried out, and by whom.

3.5 Diagnostics

22. Shared diagnostic tools and libraries provide efficiencies into the exploitation of model data. Ongoing investment will be needed to ensure timely support as new data formats, new methods of compression, and new meshes are introduced.

23. New investments will be needed to develop and/or maintain tools which can facilitate high volume data analysis, such as those which exploit parallelism, or which expedite data exploration and selection.
24. The community should seize opportunities to enhance the sharing of, and support for, diagnostic tools, recognising that shared ownership and/or development contribute to community confidence in such tools, and hence greater uptake.

3.6 Data Systems

25. It will be desirable that trans-national access to archives and compute systems be sustained in such a way as to minimise unnecessary data movement and data replication – and where possible support access to scientists from the global south in accordance with WCRP goals.
26. Sustaining access will need not only shared infrastructure, but shared infrastructure development.
27. Data volumes will continue to grow, and simulations will continue to be carried out on multiple platforms. It will be necessary to maintain distributed catalogue systems and methods to replicate data to national and international archives with co-located analysis compute.
28. Archive planning should cover transient (cache) and persistent (curated) use cases, recognizing that not all data products will be suitable for long-term curation, and different storage formats might be suitable for different use cases.
29. Even with large cache archives, not all data will be collocated for all workflows, and so software systems to support distributed analytics will need to be developed and integrated into standard tools.
30. Aspirations to share data systems, catalogues and data analytics will continue to demand common standards for data storage and metadata. Modellers should continue to use and extend the Climate Forecast conventions to maximise data re-use in accordance with FAIR principles.
31. The growing demand for climate services will lead to the need for data sharing across communities, not just within the research component of the earth system modelling community. The climate community will need to work with these other communities to ensure the appropriate services and information are available via commonly understood protocols.
32. Data users will also continue to need appropriate documentation as to how and why data were produced, and to be able to discover and report issues with the data after simulations have concluded. Systems to streamline the production and use of such information will need to be improved and maintained.

3.7 Workforce

33. In order to make the best use of new technologies it is necessary to enhance training programmes, both for new entrants into climate simulation, and for mid-career scientists. It is also necessary to maximise information sharing between European modelling groups and those carrying out data analysis.
34. Alongside training the existing workforce, there is a need to grow the size of that workforce, to support the software and scientific developments needed to sustain the delivery of climate science, while retooling models and analytic workflows for next generation computing and to make the best use of AI/ML.
35. The need for a growing workforce may involve growing by collaboration rather than by recruitment alone. Finding ways of engaging and funding already trained individuals from other disciplines to deliver precursor work for environmental science is necessary – e.g. encouraging computer science funders to support programmes which enable practical climate modelling outcomes.
36. To support the full spectrum of activities, from science to software engineering, it may be necessary to facilitate, encourage, and reward individuals who transition between science and software engineering and vice-versa.
37. In some countries and institutions, it will also be necessary to establish suitable career pathways to support permanent software engineering posts.

4. Methodology

These recommendations are based on a review of the activities and plans of the major European modelling centres carried out by the IS-ENES3 team in late 2022 and early 2023. The work builds on previous European strategies, but this version began with a series of interviews with each of the large groups (listed below), and a review of a set of large representative coordinated projects. A synthesis of the scientific drivers, key collaborations, and both bilateral and multilateral dependencies followed. That synthesis was presented to the modelling groups alongside the first version of these recommendations in March 2023.

Feedback from that meeting has been incorporated in this version, which is the first public draft. It will be made available for community feedback through May 2023, with the final version to be public in summer 2023. The underlying analysis (Lawrence et al, in preparation) will be submitted for publication at the same time.

Modelling Groups Interviewed

- French groups (IPSL, Cerfacs, Météo-France/CNRM), 20 May 2022
- CMCC, 13 June 2022

- EC-Earth groups (BSC, DMI, KNMI, SMHI), 13 June 2022
- MPI-Met & DKRZ, 14 June 2022
- UK groups (MetOffice, NCAS), 14 June 2022
- Norwegian groups (NORCE, MetNorway), 21 June 2022
- AWI, 28 June 2022

Representative European Projects Investigated

(All of which extend to the end of 2026 or beyond)

- EERIE
- OptimESM
- NextGEMS
- ESM2025
- EPOC
- OceanICE