In collaboration with

7th ENES HPC Workshop

Monday, May 9 2022 - Wednesday, May 11 2022

Abstracts

Session 1: European and International Landscape

Strengthening the European HPC communities by addressing the skills and competence level

Bastian Koller, HLRS, CASTIEL, EuroCC

In this presentation I will introduce you to the activity of the Centres of Excellence, which addresses an important European pillar: skills and competences at national and European level. The main concept behind it will be highlighted and a look at how the progress has been in the last one and a half years. Likewise, it will be shown how this activity is embedded in the European HPC ecosystem, how synergies are exploited and how the network of National Centres of Competence will continue to set itself up in the future.

Lumi - The first EuroHPC pre-exascale system

Jenni Kontkanen, CSC

The EuroHPC initiative is a joint undertaking by the European Commission and 31 countries to establish a world-leading supercomputing and data infrastructure in Europe. One of its first efforts is to install three pre-exascale supercomputers in Europe. I will discuss one of these systems, LUMI, located in Kajaani, Finland. LUMI is jointly funded and operated by the European commission and a consortium of 10 countries. When reaching its full capacity in summer 2022, LUMI is expected to become the fastest supercomputer in Europe and one of the most powerful and advanced computing systems in the world. In this talk, I will introduce the technical architecture of the LUMI infrastructure, provide a status update of the program, and discuss future plans.

ARMing the IFS: Experiments and experiences from porting the ECMWF model to Fugaku

Samuel Hatfield, ECMWF

Over the past few years, ECMWF has embarked on an ambitious program to adapt, port and run its numerical weather prediction suite, the IFS, on a range of pre-exascale supercomputers, feeding into the Destination Earth initiative. Researchers from ECMWF are now simultaneously testing the IFS on three of the top 10 supercomputers, including the number one machine, Fugaku. Fugaku is unusual in holding such a high ranking while relying entirely on CPUs, albeit the unique Fujitsu A64FX ARM-based CPU. As part of a collaboration between ECMWF and the RIKEN Centre for Computational Science, we have ported the IFS to Fugaku and have performed an initial assessment of its software ecosystem and computational performance. In this talk, I will provide an overview of these activities and results to date, including an honest discussion of difficulties encountered but also the benefits of the A64FX CPU.

Numerical Climate and Weather Modeling in China Earth System Simulator

Yongqiang Yu, LASG, Institute of Atmospheric Physics, Chinese Academy of Science

The Earth System Science Numerical Simulator Facility, named “EarthLab”, is a numerical simulation system of the main Earth systems with matching software and hardware. The peak computing power of the system will be no less than 15 trillion times per second (PFLOPS), and the total storage capacity no less than 80 PB. It can help explore the impact of each system and its interaction with the Earth system as a whole, as well as the regional environment in China; integrate simulations and observation data to improve the accuracy of forecasting; improve the prediction and projection skills for climate change and air pollution; provide a numerical simulation platform to take Earth system research in China to the top level internationally; and support China's disaster prevention and mitigation, climate change, and atmospheric environment governance, along with other major issues. The latest global climate system model named as “CAS FGOALS-f3-H” is configured with 10km and 25km resolution for oceanic and atmospheric component models respectively, and recently submitted HiResMIP experiment to the CMIP6 website. The spatial resolution of the regional high-precision simulation system will be able to reach 3 km over China and 1 km over certain key areas.

DestinE: opportunities & challenges for digital twins of the Earth System
Nils Wedi, ECMWF
The talk describes ongoing efforts to create digital replicas of the Earth as part of the European Commission's Destination Earth programme.
Global, coupled storm-resolving simulations are feasible and can contribute to building such information systems and are no longer a dream thanks to recent advances in Earth system modelling, supercomputing and the adaptation of weather and climate codes for novel computing architectures. Such simulations for example explicitly represent essential climate processes, such as deep convection and mesoscale ocean eddies, that today need to be parametrised even at the highest resolution used in global weather and climate information production. These simulations, combined with novel data-driven deep learning advances, thus offer a window into the future, with a promise to significantly increase the realism of Earth system information. Despite the significant compute and data challenges, there is a real prospect to better support global to local climate change mitigation and adaptation efforts, and complement the existing information derived with today's operational simulations in the range of 10-100 km.
Digital Twins of Earth thus encapsulate both the latest science as well as technology advances to provide near-real time information on Extremes and climate change in a wider digital environment. Here users can interact, modify and ultimately create their own tailored information. This is facilitated through complex workflows managed by ECMWF's digital twin engine that closely connects EuroHPC resources for the production of digital twin data, manages diverse data access patterns through cloud-based ancillary systems such as Eumetsat's Data Lake, and provides a diverse range of tools to facilitate user interaction and data-driven applications creating new information through ESA's user service platform. The underlying system architecture and design choices will be described and justified.

HPC Challenges for CMIP: lessons from CMIP6 and potential next steps
Jean François Lamarque, NCAR
In this presentation, I will present an overview of some of the key successes and achievements for CMIP6. I will discuss some of the early outcomes of the analysis of the CMIP6 survey, identifying themes that will be of relevance to the definition of the next phases of CMIP. I will also be discussing the current schedule of activities related to this definition.

Session 2: Mix traditional modeling with ML

Machine Learning for Weather and Climate Predictions
Peter Dueben (ECMWF)
This talk will provide a summary of the latest developments in machine learning for weather and climate predictions as discussed in the recent workshop on machine learning at the European Centre for Medium-Range Weather Forecasts (ECMWF). The talk will outline how machine learning, and in particular deep learning, could help to improve weather predictions in the coming years, name challenges for the use of machine learning, and suggest developments (research/software/hardware) that should enable the community of Earth system modelling to make quick progress.

High-Tune Explorer: a tool to accelerate model calibration based on process-oriented metrics.
F. Couvreux, Météo-France,
with F Hourdin, D Williamson, N Villefranque, R Roehrig and the High-Tune project
The development of parameterizations is a major task in the development of weather and climate models. Model improvement has been slow in the past decades, due to the difficulty of encompassing key physical processes into parameterizations, but also of calibrating the many free parameters involved in their formulation. Machine learning techniques have been recently used for speeding up the development process. While some studies propose to replace parameterizations by data-driven neural networks, we rather advocate that keeping physical parameterizations is key for the reliability of climate projections. In this paper we propose to harness machine learning to improve physical parameterizations. In particular, we use Gaussian process-based methods from uncertainty quantification to calibrate the model free parameters at a process level. To achieve this, we focus on the comparison of single-column simulations and reference large-eddy simulations over multiple boundary-layer

cases. Our method returns all values of the free parameters consistent with the references and any structural uncertainties, allowing a reduced domain of acceptable values to be considered when tuning the three-dimensional (3D) global model. This tool allows to disentangle deficiencies due to poor parameter calibration from intrinsic limits rooted in the parameterization formulations.

Skilful precipitation nowcasting using deep generative models of radar

Suman Ravuri, Google Deep Mind

Precipitation nowcasting, the high-resolution forecasting of precipitation up to two hours ahead, supports the real-world socioeconomic needs of many sectors reliant on weather-dependent decision-making. State-of-the-art operational nowcasting methods typically advect precipitation fields with radar-based wind estimates, and struggle to capture important non-linear events such as convective initiations. Recently introduced deep learning methods use radar to directly predict future rain rates, free of physical constraints. While they accurately predict low-intensity rainfall, their operational utility is limited because their lack of constraints produces blurry nowcasts at longer lead times, yielding poor performance on rarer medium-to-heavy rain events. Here we present a deep generative model for the probabilistic nowcasting of precipitation from radar that addresses these challenges. Using statistical, economic and cognitive measures, we show that our method provides improved forecast quality, forecast consistency and forecast value. Our model produces realistic and spatiotemporally consistent predictions over regions up to 1,536 km × 1,280 km and with lead times from 5–90 min ahead. Using a systematic evaluation by more than 50 expert meteorologists, we show that our generative model ranked first for its accuracy and usefulness in 89% of cases against two competitive methods. When verified quantitatively, these nowcasts are skillful without resorting to blurring. We show that generative nowcasting can provide probabilistic predictions that improve forecast value and support operational utility, and at resolutions and lead times where alternative methods struggle.

Fourier Neural Operators for Fast Weather Modeling

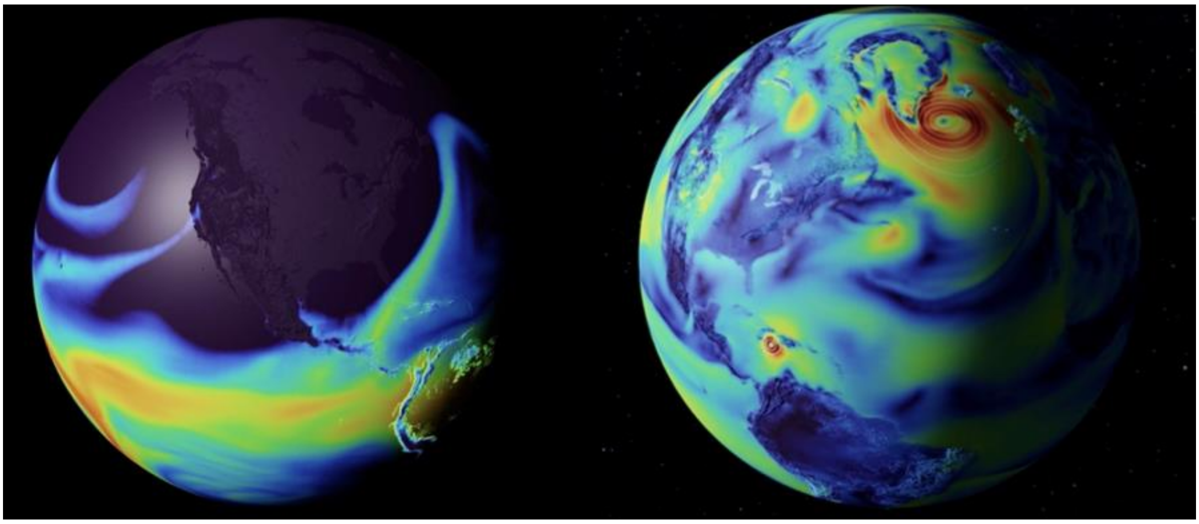
Anima Anandkumar, CalTech

Predicting extreme weather events in a warming world at fine scales is a grand challenge facing climate scientists. Policymakers and society at large depend on reliable predictions to plan for the disastrous impact of climate change and develop effective adaptation strategies. Deep learning (DL) offers novel methods that are potentially more accurate and orders of magnitude faster than traditional weather and climate models for predicting extreme events. The Fourier Neural Operator (FNO), a novel deep-learning method, has shown promising results for predicting complex systems, such as spatio-temporal chaos, turbulence, and weather phenomena. Our results show promise for large-scale DL potentially competing with state-of-the-art numerical weather prediction. The work presented here is a significant step toward building a reliable high-fidelity, high-resolution digital twin of Earth for extremes, which is widely recognized as grand challenge in the climate community.

Building Digital Twins of the Earth for NVIDIA's Earth-2 Initiative

Karthik Kashinath, Jaideep Pathak, David Hall, Thorsten Kurth, Peter Messmer, Stan Posey, Anima Anandkumar

NVIDIA is committed to helping address climate change. Recently our CEO announced the Earth-2 initiative, which aims to build digital twins of the Earth and a dedicated supercomputer, E-2, to power them. Two central goals of this initiative are to predict the disastrous impacts of climate change well in advance and to help develop strategies to mitigate and adapt to change. Here we present our work on an AI weather forecast surrogate trained on ECMWF's ERA5 reanalysis dataset. The model, called FourCastNet, employs a patch-based Vision-Transformer with a Fourier Neural Operator mixer. FourCastNet produces short to medium range weather predictions of about two dozen physical fields at 25-km resolution that exceed the quality of all related deep learning-based techniques to date. FourCastNet is capable of accurately forecasting fast timescale variables such as the surface wind speed, precipitation, and atmospheric water vapor with important implications for wind energy resource planning, predicting extreme weather events such as tropical cyclones and atmospheric rivers, as well as extreme precipitation. We compare the forecast skill of FourCastNet with archived operational IFS model forecasts and find that the forecast skill of our purely data-driven model is remarkably close to that of the IFS model for forecast lead times of up to 8 days. Furthermore, it can produce a 10-day forecast in a fraction of a second on a single GPU. The enormous speed and high accuracy of FourCastNet provides at least three major advantages over traditional forecasts: (i) real-time user interactivity and analysis; (ii) the potential for large forecast ensembles; and (iii) the ability to combine fast surrogates to form new coupled systems. Large ensembles can capture rare but highly impactful extreme weather events and better quantify the uncertainty of such events by providing more accurate statistics. The figure below shows results from FourCastNet in NVIDIA's interactive Omniverse environment. On the left we show atmospheric rivers making landfall in California in Feb, 2017. On the right is a forecast of hurricane Matthew from Sept 2016. By plugging AI surrogates into Omniverse, users can generate, visualize, and explore potential weather outcomes interactively.



Session 3: Performance

CPMIP performance metrics for CMIP6: Lessons, recommendations and next steps

Mario Acosta, BSC

The final CPMIP results were collected and published in December 2021. These results included 11 models/institutions and 32 CMIP6 configurations and has been used to create a novel database for the computational analysis of CMIP6. This activity has been useful to prove that the collection was not only a dissemination process, but also a very powerful database to analyze the computational efficiency of a model across platforms, configurations; find bottlenecks or even for a multi-model comparison. These results can be checked in the deliverable published and the peer-reviewed paper in progress.

However, we look to the future in this talk and review the complete process to do the collection and the main drawbacks found which could be improved in future collections such as CMIP7. This is a community exercise which will need the interaction and collaboration of all of us to ensure that the new database can be increased, filling the gaps encountered until now and facilitating the work for the future. Thanks to the experience, this talk includes general recommendations on how to solve these problems for future collections and why it is so important this kind of exercise.

Performance optimization in NEMO ocean model

Italo Epicoco, CMCC

The rapid advancement of new (pre-)exascale parallel architectures technologies requires a constant adaptation of the NEMO model to emerging architectures, finding solutions that guarantee performance portability on heterogeneous architectures and maintainability of the code even by people not expert in HPC. The presentation will focus on the new performance optimisations of the NEMO ocean model during the last year. HPC development strategy was aimed at reducing communication overhead, enhancing the cache memory exploitation, reducing the I/O time by means of the exploitation of XIOS library and preparing the code for a transition toward a GPU based parallelization.

The new load balancing tool in OASIS3-MCT_5.0

Eric Maisonnave, CERFACS

Updated in December 2021, the OASIS3-MCT coupler has gained new features, including a fine grain load balancing tool. This coupler has served a large community of users since 1991, both in the main climate modeling centers and smaller laboratories. Is it still useful in the age of Exascale?

The Potential of Functional Concurrency in W&C models

R. Budich, MPI-M, J. Duras, DKRZ, R. Ford, STFC

Concurrency in weather and climate models exists at different levels of granularity. Concurrency can be external to models (think ensembles) or between model components (think coupling), it can be between computation and communication (think I/O servers), it can stem from data parallelism (think distribution onto nodes or threads), or it can be intra-component functional concurrency (FC, think radiation in the atmosphere).

In the ESiWACE2 project we looked at the potential of intra-component FC to increase the amount of available parallelism to an application. This was chosen as it is not currently well exploited in Weather and Climate models. CPU-CPU, CPU-GPU and GPU-GPU examples were examined. It was found that the first two provided performance improvements, but GPU-GPU did not. We also found that one of the major obstacles to the exploitation of this form of concurrency is the lack of code modularity making it difficult to create and maintain working solutions.

In this talk we will give an introduction to FC and report on its application - not only - in the EU W&C community, based on the findings from ESiWACE2. We will highlight both the problem and the potential of FC, and argue that, whilst it may not be simple to exploit, there is a need to invest in it.

PoP Studies of Earth Sciences Codes

Jesús Labarta, BSC

The POP Center of Excellence has been performing performance analyses for applications in many domains over the past years. The talk will briefly summarize some of the assessments done in the area of weather/climate codes as part of the POP activity and some other cooperations in the domain.

Beyond that I will introduce the EPI RISC-V vector architecture and the Software Development Vehicle that is allowing us to evaluate the architecture and produce co-design insight using some climate dwarf miniapps.

Recent Atlas library developments for Earth system modelling

Willem Deconinck, ECMWF

ECMWF has the strategy to run ECMWF's Integrated Forecasting System (IFS) -- or at least some of its Earth sytem model components -- on non-traditional hardware such as GPUs. In this strategy, the ECMWF Atlas library plays a central role to manage data structures, distributed parallelisation, and memory spaces.

The Atlas library abstracts field data allocations to backends specifically for dedicated hardware, and provides data synchronisation capabilities between host CPU memory spaces and GPU device memory. Orthogonally, IFS consists of various Earth system model components such as atmosphere, radiation, ocean, ocean waves. These components may each operate on different grids and use different parallel distributions. Adding GPU device memory spaces to this mix is inevitably making the coupling of these components more challenging. ECMWF therefore aims to integrate Atlas deeper in each Earth system model component, and thus take advantage of a common data structure library to efficiently interpolate fields between each component.

This presented talk will elaborate on the recent Atlas developments to bring us closer to our ambitious goals.

On the energy costs of data production, data transfer and data storing

Jean-Claude André, CERFACS

European climate modelling groups have been involved in the production of CMIP6 simulations that have contributed to the 6th IPCC assessment report. The estimated amount of compute resources that have been necessary represents only 50% of the total effort. Production of the total 50 PB of data corresponds to almost 5.000 million of core hours, *i.e.* to an electric consumption of about 10.000 MWh. Energy costs of data exchange between groups, and of data storing at either locally of centralized data centers, are much more difficult to estimate, probably amounting to an additional few thousands of MWh. Converting these energy costs in carbon footprints remains to be done, with the additional difficulty that it strongly depends upon the way electricity is being produced in the various European countries.

Session 4: Heterogeneous architectures (accelerators)

Preparing ICON for heterogeneous architectures - Experiences and the way forward
Claudia Frauen, DKRZ
Directive-based approaches like OpenACC and OpenMP provide a relatively easy way to port large model codes to GPU-based systems. This approach was also successfully applied to the atmospheric component of the weather and climate model ICON. However, this is not sufficient for the development of an ICON-based earth system model capable of resolving global oceanic and atmospheric coupled circulation systems on kilometer-scales with a throughput of one simulated year per day on future exascale HPC-systems, which is a central goal of the German national project WarmWorld. To achieve this, a transformation of the ICON software towards an open, scalable, modularized and flexible code is needed such that independent development (both scientific and informatics) will be enabled.

PSyclone in Met Office: Evolution and revolution
Iva Kavcic, Met Office
PSyclone is a domain-specific compiler and source-to-source translator developed for use in finite element, finite volume and finite difference codes used in Earth System Models. In essence, it uses domain-specific knowledge to construct a representation of the target code and allows the HPC expert to transform this representation so as to add various forms of parallelisation (distributed memory, OpenMP threading, OpenMP offload, OpenACC). This talk will give an overview on how PSyclone is applied to models used in and developed by the Met Office, from working with existing code in the NEMO ocean model to interdependent development with the new MO LFRic weather and climate modelling system.

Accelerating tracer transport in FESOM-2 with GPU's
Gijs van den Oord, Netherlands eScience center
Within the ESiWACE-2 service on porting applications to pre-exascale machines, we have collaborated with the FESOM-2 team to accelerate parts of their model on GPU's. FESOM-2 is a finite-volume ocean and sea-ice model based on unstructured meshes. We have used the OpenACC programming model to speed up the transport of tracers in FESOM-2. In this talk, I will share the results of this effort, describe our collaboration with the FESOM team and present some technical aspects of the implementation. Finally, I will iterate on the lessons learned and the road ahead for FESOM-2 towards exascale.

CAMP First GPU Solver: A Solution to Accelerate Chemistry in Atmospheric Models
Christian Guzman Ruiz, Barcelona Supercomputing Center
Chemistry is usually one of the main bottlenecks when this component is coupled to an atmospheric model. We aim to achieve an efficient GPU version of the chemical module Chemistry Across Multiple Phases (CAMP). CAMP is a solver library which is on deployment to be used as a library for any chemical component in the future. We obtain up to 36x speedup from the CPU single-thread version and up to 3x against the MPI implementation using a full node (40 physical cores). Our approach can be a good alternative to speed up the chemistry solvers for atmospheric models or even as a novel approach for other GPUs porting.

Preparing IFS for HPC accelerators via source-to-source translation
Michael Lange, ECMWF
The need to fully exploit the advantages of modern accelerators in HPC architectures plays a vital role in achieving the next step change in predictive skills for weather and climate models. However, the diversification of HPC hardware continues and incurs a recurring need to adapt and transform existing model software to new programming models, which is becoming increasingly impractical using a single code base. All current strategies tackling this issue involve some form of abstraction that separates numerical algorithms from hardware-specific implementation. ECMWF is aiming to achieve both compatibility and performance portability for accelerators and future architectures through a combination of DSLs, domain-specific libraries and bespoke source-to-source translation tools that allow an incremental adaptation of the code base alongside scientific development.
In this talk we will describe algorithmic components of the Integrated Forecasting System (IFS) and highlight key elements of our roadmap for adapting them to GPU architectures. We discuss how a combination of flexible data structures, an extended use of library interfaces and the use of source-to-source translation tools is envisaged to allow the incremental adaptation of the code base. The second part will focus on Loki, an in-house developed

tool that allows bespoke source-to-source transformations to be devised to adapt individual model components to novel programming paradigms or community-driven DSLs.

Enabling large scale modeling on GPU accelerated nodes for NCAR's next supercomputer Derecho

Thomas Hauser, NCAR

The upcoming NCAR Derecho supercomputer will provide 20% of its sustained computing capability from nodes with four NVIDIA A100 graphics processing units, with the remainder coming from dual socket nodes with AMD EPIC 7763 Milan processors. This presentation will describe NCAR's collaborative approach in getting codes ready for the accelerated scientific discovery (ASD) program. I will provide preliminary porting results of three different applications and how the scientific objectives motivate and influence the GPU porting approach.

E3SM's C++ based GPU strategy and latest performance

Mark Taylor, Sandia National Laboratories

I will give an overview of the Energy Exascale Earth System Model (E3SM) project's work porting our atmosphere components to GPUs. We are targeting the U.S. Department of Energy's upcoming GPU based Exascale computers. E3SM is developing a global cloud resolving model (SCREAM) and a superparameterized version of the E3SM atmosphere (E3SM-MMF). SCREAM is written nearly entirely in C++, with Kokkos used to abstract the execution model for on-node parallelism. For the E3SM-MMF, we make use of the fact that the computational work is nearly all contained in the superparameterization (SAM) and the radiation package (RRTMGP), both of which we have rewritten in C++ in order to support GPUs. For SAM and RRTMGP, we used YAKL (Yet Another Kennel Launcher) for on-node parallelism and performance portability. We have found the C++ approach, with ether Kokkos or YAKL, to be more robust and better supported then a Fortran+directives based approach across several different GPUs (NVIDIA, AMD and Intel). For our C++/Kokkos code, we have also worked to maintain Fortran-level performance on CPU systems through the use of "packs" in order to ensure proper vectorization.

Session 5: Data Workflow

Nobody needed all those bits anyway: compressing atmospheric data into its real information content

Milan Klöwer, Oxford

Hundreds of petabytes of data are produced annually at weather and climate forecast centres worldwide. Compression is inevitable to reduce storage and to facilitate data sharing. Current techniques do not distinguish the real from the false information in data. We define the bitwise real information content from information theory for climate data which objectively suggests a level of required precision to be retained in lossy compression. Most atmospheric variables of the Copernicus Atmospheric Monitoring Service (CAMAS) contain less than 7 bits of real information per value, which are also highly compressible due to spatio-temporal correlation. Rounding bits without real information to zero facilitates lossless compression algorithms and encodes the uncertainty within the data itself. Compression errors are bounded by the rigid error bounds of floating-point numbers, minimising compression artefacts. The entire CAMS data is compressed by a factor of 17x, relative to 64-bit floats, while preserving 99% of real information. Combined with 4-dimensional compression to exploit the spatio-temporal correlation, factors beyond 60x are achieved without an increase in forecast errors. A data compression Turing test is proposed to optimise compressibility while minimising information loss for the end use of weather and climate forecast data.

Fostering lossy compression in the European Earth System Modelling community: SZ compressor and XIOS I/O server as a case study

Xavier Yepes, Barcelona Supercomputing Center

One-paragraph abstract: Earth system models (ESMs) will progressively take advantage of the upcoming exascale era, but their current data management systems are not prepared yet to deal with the exponential data growth. Default lossless compression filters, such as gzip in HDF5, do not provide a good trade-off between size reduction and computational cost. We therefore consider using lossy compression filters that may allow reaching high compression ratios and enough compression speed to considerably reduce the I/O time while keeping high accuracy. As a case study, we are exploring the feasibility of using the SZ lossy compressor developed by the Argonne National Laboratory (ANL) to write highly compressed NetCDF files through the XML Input/Output Server (XIOS), an MPI parallel I/O server with inline post-processing developed by the Institute Pierre Simon

Laplace (IPSL). In particular, the Open Integrated Forecast System (OpenIFS) is used with XIOS, an atmospheric general circulation model.

Data-Centric workflows in Exascale Weather Forecasting
Tiago Quintino, Domokos Sarmany, Simon Smart, James Hawkes, Emanuele Danovaro, Olivier Iffrig, Nicolau Manubens, Baudouin Raoult, Peter Bauer
ECMWF operational weather forecast is a highly data intensive HPC workflow that generates massive amounts of I/O in short bursts, accumulating to tens of TiB in hourly forecast cycle windows. From this output, millions of user-defined daily products are generated and disseminated to member states and commercial customers all over the world. These products are processed from the raw output of the IFS model, within the time critical path and under strict delivery schedule.
Over the last 8 years, multiple EU funded projects such as NextGenIO, MAESTRO, Lexis, to name a few, have promoted a faster adoption of novel IO technologies. A core central concept in all these projects has been 'data-centric workflows', which focus on optimising the use and usefulness of the data, close to its point of origin. A comprehensive software stack has been developed that supports this vision, including packages such as a domain specific object-store (FDB) and a purposefully built, multiplexing IO-server (MultIO).
A new phase of EU investment into this area is being ushered in by the Destination Earth programm. During its first phase, two high resolution Digital Twins will be developed: (1) a kilometer scale Global Weather Extremes forecast and (2) a high-resolution climate change and adaptation digital twin, which combined are estimated to generate around 1 PiB/day.

We present the challenges ECMWF is facing, in particular with upcoming Destination Earth, and the latest developments in model I/O, product generation and data storage. We show how ECMWF is reworking our operational workflows to adapt to forthcoming new architectures and memory-storage hierarchies, while building the API's that will empower the users to fully utilise rich, dense Exascale datasets.

ExCALIData: Exascale I/O & Storage and Workflow
Grenville Lister
“Redesigning codes and workflows to take advantage of exascale simulation requires addressing I/O and workflow problems which arise throughout a sequence of activities that may begin and end with deep storage and will involve both simulation and analysis phases”. We describe the ideas behind the two complementary elements of the ExCALIData project, namely, ExCALIStore (I/O & Storage) and ExCALIWork (Workflow), and report some initial progress in developments in active storage, ensemble workflows, and hardware solutions.
https://excalibur.ac.uk/projects/excalidata/

Semantic access to gridded weather data based on zarr
Gabriela Aznar Siguan, MeteoSwiss, With Néstor Tarin Burriel, Philipp Falke, Matthieu Bernard
The enhancement of weather forecasts using machine learning or statistical approaches requires a large archive of gridded data extending to several years in the past. This data is heterogeneous, comprising fields with high resolution in space and time of observations such as satellite and radar and outputs of probabilistic numerical weather prediction models. At MeteoSwiss, we have been developing a unified multi-dimensional gridded data service to facilitate data access and analysis for developing and training post-processing methods. The database must allow the slicing and retrieval of the data along various dimensions to allow for different machine learning applications and evaluations.
GrideFix stores gridded data in a data store using the zarr format with a tailored storage layout implemented through zarr groups. All zarr metadata are hold in a PostgreSQL database for maintaining access speed even on large archives. The storage layout allows for drip feeding data and for rolling update along the main time axis. A core library manages the storage component through xarray Datasets and sustains the import, export and catalogue services. The services are cloud-native, allowing by construction to scale horizontally as well as vertically by relying on dask threads. The export service implements a REST API for retrieving data through the OPeNDAP protocol, which is natively supported by the NetCDF library, whilst the catalogue REST API provides a high-level interface to the metadata store. To provide maximum flexibility for storing diverse data no hierarchy is imposed, instead each dataset is identified by a unique set of tags. The dataset variables follow the CF naming convention, making the query of the same physical quantity from different data sources straightforward.

Towards HPC and Big Data convergence for climate analysis at scale

Donatello Elia, CMCC Euro-Mediterranean Centre for Climate Change

“The ever-growing volume and complexity of data in the last two decades brought about a radical transformation in the analysis process within many scientific domains, as these become increasingly dependent on efficient tools for data handling and value extraction. The integration of High-Performance Computing and data analytics represents an invaluable opportunity to deliver novel and scalable High Performance Data Analytics (HPDA) solutions that can effectively cope with these data. In this context, the Ophidia framework, developed at CMCC, aims to provide a scalable HPDA solution for scientific applications. This talk will address some of the main challenges and trends towards HPDA at scale for eScience, with a focus on the climate science domain, and it will illustrate some of the latest developments for the Ophidia framework in this direction."