Toward large scale distributed experiments for climate change data analytics in the Earth System Grid Federation (ESGF) eco-system

S. Fiore[1], D. Williams[2], V. Anantharaj[3], S. Joussaume[4], D. Salomoni[5], S. Requena[6], G. Aloisio[1,7]

[1]*Euro-Mediterranean Center on Climate Change Foundation, Italy and ENES*
[2]*Lawrence Livermore National Laboratory, Livermore, California, USA*
[3]*Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA*
[4]*CNRS, France and ENES*
[5]*INFN Division CNAF (Bologna), Italy*
[6]*GENCI, France*
[7]*University of Salento, Italy*

Introduction

The increased models resolution in the development of comprehensive Earth System Models is rapidly leading to very large climate simulations output that pose significant scientific data management challenges in terms of data sharing, processing, analysis, visualization, preservation, curation, and archiving[1,2,3]. In this domain, large scale global experiments for climate model intercomparison (CMIP[4]) have led to the development of the Earth System Grid Federation (ESGF[5]), a federated data infrastructure involving a large set of data providers/modelling centres around the globe, which includes the European contribution - regarding the ENES[6] community – through the IS-ENES project.

From an infrastructural standpoint, ESGF provides a production-level support for search & discovery, browsing and access to climate simulation data and observational data products. ESGF has been serving the Coupled Model Intercomparison Project Phase 5 (CMIP5) experiment, providing access to 2.5PB of data for the IPCC[7] AR5[8], based on consistent metadata catalogues. In such a context, running a climate model intercomparison data analysis experiment is very challenging, as it requires the availability of large amount of data (multi-terabyte order) related to multiple climate models simulations as well as scientific data management tools for large-scale data analytics.

This paper presents (i) key challenges regarding large-scale climate data analysis, (ii) a paradigm shift for the climate change community towards the exascale era with a strong focus on data intensive facilities, high performance analytics, and server-side approaches, and (iii) a real testbed across US and Europe (in the context of the H2020 INDIGO-DataCloud project) joining HPC, Cloud and Big Data into a novel Platform-as-a-Service (PaaS) architecture serving multiple research communities and in particular, for the climate change one, addressing current challenges, issues and requirements related to the multi-model ensemble analysis of CMIP5 data.

Key issues and challenges regarding climate data analysis

Presently, ESGF provides a large-scale, geographically distributed, data-sharing infrastructure. In the current environment, the setup of a data analysis experiment requires that all the needed climate datasets must be downloaded from the related ESGF data nodes on the end-user's local machine. Such a preparatory step represents a strong barrier for climate scientists, as the data download can take (depending on the amount of data needed by the experiment, i.e a multi-model experiment) a significant amount of time. Moreover, the client-side nature of the current approach requires end-users to have system management/ICT skills to install and update all the needed data analysis tools/libraries on their local machines. Yet, another point relates to the complexity of the data analysis process itself and the need for end-to-end workflow support solutions; indeed, analysing large datasets involves running tens/hundreds of analytics operators in a coordinated fashion. This is usually done via scripts (e.g. bash) on the client side (instead of workflow tools) and requires climate scientists to take care of, implement and replicate workflow-like control logic aspects (which are error-prone too) in their scripts, along with the expected application-level part. Finally, the large volumes of data

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[1] J. Dongarra, P. Beckman, T. Moore, P. Aerts, G. Aloisio, J. C. Andre, D. Barkai, J. Y. Berthou, T. Boku, B. Braunschweig, F. Cappello, B. M. Chapman, X. Chi, A. N. Choudhary, S. S. Dosanjh, T. H. Dunning, S. Fiore, A. Geist, B. Gropp, R. J. Harrison, M. Hereld, M. A. Heroux, A. Hoisie, K. Hotta, Z. Jin, Y. Ishikawa, F. Johnson, S. Kale, R. Kenway, D. E. Keyes, B. Kramer, J. Labarta, A. Lichnewsky, T. Lippert, B. Lucas, B. Maccabe, S. Matsuoka, P. Messina, P. Michielse, B. Mohr, M. S. Mueller, W. E. Nagel, H. Nakashima, M. E. Papka, D. A. Reed, M. Sato, E. Seidel, J. Shalf, D. Skinner, M. Snir, T. L. Sterling, R. Stevens, F. Streitz, B. Sugar, S. Sumimoto, W. Tang, J. Taylor, R. Thakur, A. E. Trefethen, M. Valero, A. van der Steen, J. S. Vetter, P. Williams, R. Wisniewski, K. A. Yelick: "The International Exascale Software Project roadmap". International Journal of High Performance Computing Applications (IJHPCA) 25(1): 3-60 (2011), ISSN 1094-3420, doi: 10.1177/1094342010391989.

[2] European Exascale Software Initiative roadmap - http://www.eesi-project.eu/pages/menu/project/eesi-1/publications/final-report-recommendations-roadmap.php

[3] PRACE – The Scientific Case for High Performance Computing in Europe 2012-2020 - http://www.prace-ri.eu/IMG/pdf/prace_-_the_scientific_case_-_full_text_-.pdf

[4] The CMIP framework (established by the Working Group on Coupled Modelling (WGCM) under the World Climate Research Programme (WCRP)) enables a diverse community of scientists to analyse GCMs in a systematic fashion, a process that serves to facilitate models improvement.

[5] Earth System Grid Federation - http://esgf.llnl.gov

[6] ENES European Network for Earth System Modelling

[7] Intergovernmental Panel on Climate Change – http://www.ipcc.ch

[8] IPCC Fifth Assessment Report - https://www.ipcc.ch/report/ar5/

and the strong I/O requirements pose additional challenges related to performance, which requires a substantial re-design effort at the storage level both in terms of I/O interfaces and physical storage layout to address current issues.

A paradigm shift for data analysis to face the exabyte era

The issues mentioned in the previous section are going to get worse and unmanageable in the exabyte era. To address and overcome them, a paradigm shift must be envisioned. A different approach based on (i) data-intensive facilities running high-performance analytics frameworks jointly with (ii) server-side analysis capabilities, should to be explored.

Data intensive facilities (representing the counterpart to the HPC eco-system for climate models simulations) close to the different storage hierarchies will be needed to address high-performance scientific data management. On top of them, parallel applications and in-situ and in-transit frameworks[9] for big data analysis (exploiting MPI, OpenMP, MapReduce paradigms as well as machine/deep learning new techniques for features detection/extraction) should provide a new generation of "tools" for climate scientists. In such a landscape joining HPC and big data, deep learning methods and cloud technologies could help on deploying in a flexible and dynamic manner analytics applications/tools as containers or virtual machines, thus enabling highly scalable and elastic scenarios in both private clouds and cluster environments.

Server-side approaches will intrinsically and drastically reduce data movement. Download will only relate to the final results of an analysis (e.g., images, maps, reports and summaries typically megabytes or even kilobytes). Such an approach would strongly reduce the amount of data downloaded on the client side as well as the complexity related to the analysis software to be installed on client machines. Moreover, as server-side approaches will benefit from data locality, the geographic datasets distribution will require specific tools or frameworks to orchestrate multi-site experiments to support multi-model ensemble analysis experiments. So, end-to-end systems will be needed to handle such kind of aspects. Yet, server-side approaches will also spur development of new client software like visualization tools, decoupling the front-end aspects about data presentation, from the back-end ones about data analysis. Moreover, they will also enable managing raw data, intermediate products, final outputs, workflows, lineage information and users sessions on the back-end, thus allowing (through the sharing of this information) climate scientists to: (i) resume sessions from different client locations, (ii) perform collaborative experiments, (iii) re-use partial/final results across experiments, (iv) re-produce past experiments, etc. Finally, server-side approaches will also require a strong effort on interoperability and standard interfaces in order to build highly interoperable tools and environments for climate data analysis. In this regard, both the Research Data Alliance (RDA) and ESGF are already working on these topics at different levels with valuable contributions on big data analytics, array-databases, persistent identifiers, standard interfaces for server-side processing, etc.

A real case study on multi-model ensemble climate data analysis

In the context of the EU H2020 INDIGO-DataCloud project[10,11], a use case on *climate models intercomparison data analysis* is being implemented to address multiple classes of data analysis (anomalies analysis, trend analysis, and climate change signal analysis). In particular, as opposed to the current scenario based on the three-step workflow (search & discovery, data download, and client-based sequential data analysis), the INDIGO-DataCloud architectural solutions aim at providing a dynamic approach relying on server-side and high performance big data frameworks jointly with two-level workflow management systems realized at the PaaS level via a Cloud infrastructure.

Such a solution is the result of a strong requirements analysis carried out in the first months of the project that can be summarized in the following key points: efficiency, flexibility, interoperability, easy-to-use environment, and end-to-end analytics support.

The three classes of experiments are strongly related to multi-model ensemble analysis and require the access to one or more (distributed) data repositories (e.g. managed by ESGF data nodes), as well as running complex analytics workflows with multiple operators. Such workflows are being designed jointly with climate scientists to fully address the scientific challenges. Workflows also include the execution of already existing tools widely adopted by the community for data processing and visualization.

Worth of mentioning in the proposed use case, is the two-level workflow strategy based on Kepler[12] (Workflow management system - WfMS) and Ophidia[13] (big data analytics framework for climate change) which allows running geographically distributed, scientific data analysis workflows, like the ones implemented in the proposed use case. The

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[9] http://www.eesi-project.eu/wp-content/uploads/2015/05/EESI2_D7.3_Final-report-on-EESI2-exascale-vision-roadmap-and-recommendations.pdf

[10] INDIGO-DataCloud - https://www.indigo-datacloud.eu

[11] Davide Salomoni, Isabel Campos Plasencia, Luciano Gaido, Giacinto Donvito, P. Fuhrman, Jordi Marco, A. Lopez-Garcia, Pablo Orviz, Ignacio Blanquer, Germán Moltó, Marcin Plóciennik, Michal Owsiak, Michal Urbaniak, Marcus Hardt, Andrea Ceccanti, B. Wegh, J. Gomes, Mário David, Cristina Aiftimiei, L. Dutka, Sandro Fiore, Giovanni Aloisio, Roberto Barbera, Riccardo Bruno, Marco Fargetta, Emidio Giorgio, S. Reynaud, L. Schwarz: INDIGO-Datacloud: foundations and architectural description of a Platform as a Service oriented to scientific computing. CoRR abs/1603.09536 (2016)

[12] The Kepler project - https://kepler-project.org/

[13] S. Fiore, A. D'Anca, C. Palazzo, I. T. Foster, D. N. Williams, G. Aloisio, "Ophidia: Toward Big Data Analytics for eScience", ICCS 2013, June 5-7, 2013 Barcelona, Spain, ICCS, volume 18 of Procedia Computer Science, page 2376-2385. Elsevier, 2013

two-level strategy joins the main benefits of a coarse-grain approach for multi-site tasks orchestration with a fine-grain one specifically designed for data analytics experiments[14]. More specifically:
a) the Kepler general-purpose workflow management system is exploited in this use case to orchestrate multi-site tasks (level 1) related to the multi-model, ensemble part of the experiment;
b) the Ophidia framework is adopted at the single-site level to orchestrate the site-specific analytics workflow (level 2), related to the single-model parts of the experiment. Such workflow will run on multiple sites and will include tens of data processing, analysis, and visualization operators in Ophida, while acting at the same time as a single level-1 task in Kepler.
A geographically distributed testbed involving three ESGF sites (LLNL, ORNL and CMCC) represents the test environment for the proposed solution that is being applied on CMIP5 datasets. Through the INDIGO-DataCloud PaaS software stack, the Ophidia clusters and the Kepler WfMS can be instantiated and deployed on-demand on the testbed sites using standard Cloud interfaces. This results in the availability of dynamically distributed interactive and batch scenarios interoperating with existing ESGF tools and supporting optimization of the various classes of data analysis, performed via the integration of data and compute resources and proper exploitation of data locality. Preliminary results are already available on the initial prototype, while a full test case implementation will be available during Summer 2016.

Related initiatives and projects
Some relevant related initiatives and projects strongly linked to the case study presented in this work, and that are expected to provide valuable feedback, are: (i) the Center of Excellence on Weather and Climate Simulations in Europe (ESiWACE[15]) that aims at addressing, among the others, optimizations at the storage level and end-to-end workflow support through a co-design based approach and (ii) the European Extreme Data & Computing Initiative (EXDCI[16]) whose objective is to coordinate the development and implementation of a common strategy for the European HPC Ecosystem joining the expertise of the two most significant HPC bodies in Europe, PRACE[17] and ETP4HPC[18].

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[14] Marcin Plociennik, Sandro Fiore et al, "Two-level dynamic workflow orchestration in the INDIGO-DataCloud for large-scale, climate change data analytics experiments", ICCS2016 Conference, San Diego, California, USA, 6-8 June, 2016 [to appear].
[15] ESiWACE - https://www.esiwace.eu/
[16] EXDCI - https://exdci.eu/
[17] PRACE - http://www.prace-ri.eu
[18] ETP4HPC - www.etp4hpc.eu/en/sra.html