REQUEST FOR A SPECIAL PROJECT 2023–2025

MEMBER STATE: Spain

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BSC: Iria Ayan
ECMWF: Marcus Koehler, Anna Agusti-Panareda, Gianpaolo Balsamo

Project Title: OpenIFS Modeling of the Atmospheric Carbon Cycle

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SPNLPETE**	
Starting year: (A project can have a duration of up to 3 years, agreed at the beginning of the project.)	2023	
Would you accept support for 1 year only, if necessary?	YES	

Computer resources required for 2023-2025: (To make changes to an existing project please submit an amended version of the original form.)		**2023**	**2024**	**2025**
High Performance Computing Facility	(SBU)	21M	29M	0
Accumulated data storage (total archive volume)[2]	(GB)	15000	15000	

Continue overleaf

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Extended abstract

The carbon dioxide (CO2) balance of the atmosphere is undergoing rapid change. While CO2 emissions are expected to increase, then peak, and subsequently decrease as commitments to the Paris Agreement take hold, the fate of the current sink of CO2 in oceans and biosphere (together ~4 PgC/yr) is unclear. Ongoing warming and fertilization might boost photosynthesis in the land biosphere and expand forest area polewards. But the impact of droughts, loss of forest resilience, the intensified cycle of precipitation and evaporation, and increase in respiration and fires might tip the balance and turn current carbon sinks into sources. The uncertainty that stems from our incomplete understanding of the carbon cycle hampers climate projections on decadal scales, but also complicates the attribution of observed CO2 mole fraction variations to various anthropogenic sources, and to (managed) land-use at the national scale. Both are an integral part of our joint efforts under the Paris Agreement.

Simulating the global carbon cycle at multi-decadal timescales is playing an increasingly important role in European research projects related to climate mitigation, climate neutrality and negative emission technologies, such as the recently awarded Horizon Europe projects RESCUE and OptimESM. These projects use at their core Earth System Models with interactive CO2 driven by CO2 emissions and land and ocean carbon cycle components at their core.

Numerical modelling is key in climate predictions and driver attribution of atmospheric CO2 change, and in both, ECMWF's Integrated Forecast System (IFS) is set to play a major role. In addition to being the world-leading Numerical Weather Prediction (NWP) system, IFS has become the dynamical core of the EC-Earth climate model v3 and its successor v4 which is built and maintained by the EC-Earth consortium. IFS similarly forms the core of the Copernicus Atmospheric Monitoring System (CAMS) and its evolving Monitoring and Verification System (MVS) for greenhouse gases.

Active IFS development for GHG modelling by ECMWF staff in projects such as CHE, VERIFY, CoCO2, EYE-CLIMA, AVENGERS, PARIS, and CORSO is strengthened by a large research community working with similar, or closely related, atmospheric transport models such as TM3/TM5. Upcoming "Invitations to Tender" that reinforce ECMWFs activities under the Copernicus umbrella are strongly geared towards expanding the utility of IFS for greenhouse gas (and especially CO2) modelling, suggesting a possibly fast growth of IFS-GHG modelling activities, and its external research community. The proposed project is therefore highly relevant to ECMWF's objectives.

A subset of this community has started to work with OpenIFS, the licensed academically-oriented release of the IFS code. As core of the upcoming EC-Earth4, and with its latest release closely following the IFS operational cycle (**next major release is planned to be based on 47r3)**, the OpenIFS platform is an ideal platform to test and develop a new modelling capacity. This includes land-atmosphere feedbacks involving the terrestrial biosphere, land-use change (LUC) scenarios that include short- (aerosol) and long-term (CO2) climate impacts, and coupled carbon-water exchange for climate modelling. Further, this emcompasses multi-tracer simulations, fast chemistry-schemes, ensemble predictions, and data assimilation (outside the scope of ECMWF's NWP setting) to obtain enhanced Monitoring Verification System (MVS) capacity. These applications all benefit from a collaborative development initiative by a strong community focused on GHG modelling using OpenIFS:

(1) CO2 as a long-lived tracer with high variability on diurnal to interannual timescales and therefore a unique challenge to simulate: both mass-conservation (over time scales of years) and gradient-conservation (on time scales of hours) is needed. With both climate and MVS applications in one team, best practices and numerical improvements can quickly be shared, while preventing one community from sacrificing features that are key to the other.

(2) Sharing code developments, but also evaluation tools, input datasets, and capacity to for example nudge to ERA5 reanalysis, or perform ensemble simulations with realistic stochastic forcings on key carbon cycle processes, will save our communities time, help us gain efficiency, and minimize redundancy in our efforts.

(3) Expertise to perform GHG simulations across the communities has developed independently with knowledge on long-term simulations, short-term chemical interactions and satellite data of CO2 precursors, and data assimilation of in-situ observations distributed across the groups. Consolidating this knowledge is relatively easy as individual researchers have already established connections or collaborated.

(4) Both communities share a close connection to ECMWF staff involved in OpenIFS, and development of IFS's greenhouse gas modelling capacity. Given the large commitments of ECMWF and their stretched resources that are maximally targeting the Copernicus deliverables, one bridge to the academic community across which communication and collaboration takes place will greatly enhance efficiency of all teams involved.

In 2022 this sub-community has taken a first step towards self-organization, using an ECMWF Special Project with one year of support to:

(a) Organize regular exchange of information through monthly project meetings, and work together towards shared use of OpenIFS for CO2 simulations

(b) Install and test various OpenIFS versions, including the one within EC-Earth4, on ECMWF's computing platforms **(including CCA and the new Atos BullSequana XH2000-ATOS)**, as well as national supercomputing facilities (Spain, Netherlands).

(c) Engage the ECMWF community working on carbon cycle studies with IFS, obtain formal training on OpenIFS, and share project components.

This proposal is a next step in the development of our community, and to expand our shared modeling capacity. The renewed support of ECMWF in the form of a follow-up special project would boost our efforts.

In the next sections we will expand on the scientific and technical details of the efforts we aim to synthesize.

The team

The project will involve researchers at the Barcelona Supercomputing Center (BSC) in Spain (Tourigny, Ayan), Wageningen University & Research (WUR) in the Netherlands (Peters, van den Berg) as well as Utrecht University (UU, Koren) and the Max-Planck-Institute for Biogeochemistry (MPI-BGC) in Jena, Germany (Winkler). These groups have been in close contact on the proposed development over the past 12 months, leading to the creation of the OpenIFS/CC (OpenIFS/CC :

Carbon Cycle) group hosted on the ECMWF CONFLUENCE infrastructure at https://confluence.ecmwf.int/pages/viewpage.action?pageId=226496552.

The three groups are supported by expertise from ECMWF (Koehler) and is in close contact with ECMWF's greenhouse gas modelling experts (Agusti-Panareda, Balsamo, Koffi, Luca, Panagiotis, Bousserez) who will continue to provide advice and scientific feedback to the team but cannot commit to investing hours.

We previously proposed a small one year project for 2022 (in progress) to be followed by a larger proposal (this request) with its scoping based on preliminary results. ***In addition, this coincides with the expected major upgrade of OpenIFS to 47r3 which is the target version for our major developments, whereas OpenIFS 43r3v2 will be used for initial developments***. We note that most of our team members have prior experience on ECMWFs computing platforms (including CCA, TEMS and ATOS), and have access through earlier collaborations and special projects (i.e. Etienne Tourigny, special project spesiccf).

Projects targeted in 2023-2024

In the lead-up project of 2022, the BSC team has set up reference IFS 43R1 and 43R3 experiments with CO2 tracers, anthropogenic emissions, CTESSEL fluxes, ocean fluxes and biomass burning fluxes using the prepIFS infrastructure, with the help of Anna Agusti-Panareda. These reference runs were done to identify the proper namelist configuration and initial and forcing files required to run OpenIFS with CO2 tracers enabled.

Moreover, BSC has successfully built and run the EC-Earth4 4.0 release on the BSC's Marenostrum4 HPC, as well as the trunk version on both Marenostrum4 and ECMWF's ATOS HPC, which includes an update to OpenIFS 43r3v2 (with improved mass fixers), NEMO 4.2 and oasis3-mct-5.0 (with python api required for the python/oasis forcing reader).

Based on this experience at BSC, it was decided during the final meeting of the OpenIFS/CC project year 2022 to collectively use the EC-Earth4 framework to conduct our follow-up experiments. This recognizes that also our other plans would benefit from EC-Earth4 specific features such the access to AMIP SST/SIC forcings, CMIP6 forcings, a flexible python/oasis-based forcing reader adaptable to various forcing sources, e.g. input4MIPS (for CMIP6), GridFED emissions and biogenic CO2 fluxes from CarbonTracer Europe, replacing the reading of grib files in OpenIFS. The components together comprise the EC-Earth4-CC-lite configuration in which the CO2 fluxes from the land vegetation (LPJ-GUESS) and ocean (NEMO/PISCES) biogenic components in the full EC-Earth4-CC configuration are replaced with fluxes from from CarbonTracer Europe (see Figure 1).

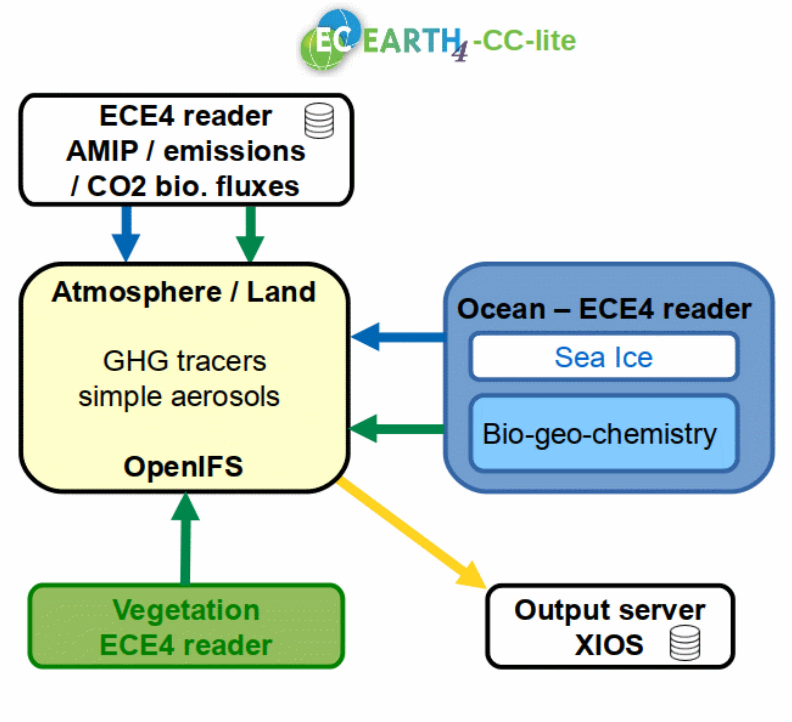

Figure 1 - Diagram of the EC-Earth4-CC-lite configuration.

Subproject 1: CO_2 transport in coupled climate model with OpenIFS using the EC-Earth4 framework (BSC)

The Barcelona Supercomputing Center (BSC) Earth Sciences department, along with colleagues from KNMI, Lund University and SMHI has been actively involved in the development of EC-Earth3-CC, the carbon cycle version of EC- Earth3 (Döscher et al, 2021). The EC-Earth3-CC model comprises the IFS atmospheric model, NEMO ocean model with LIM3 sea-ice model and PISCES ocean biogeochemistry model, LPJ-GUESS dynamic vegetation model and TM5 for the transport of atmospheric CO2, used in the emission-driven version of the model. The TM5 model is used for transport of CO2 as a passive tracer, ensuring mass conservation during centuries-long simulations. This was done because the version of IFS (cy36r4) is quite old and does not include mass-conserving transport of CO2. This results in a considerable slowdown of the coupled system, leading to a 50% decrease in model throughput.

The EC-Earth3-CC model has been used for the CMIP6, C4MIP and LUMIP CMIP exercises and is used in a number of H2020 projects in which the BSC is involved in, such as 4C (Carbon-Climate Interactions in the Current Century) and LANDMARC (Land Use Based Mitigation for Resilient Climate Pathways). Within the 4C project, the BSC has implemented a near-term prediction of the carbon cycle, building upon the successful decadal forecasting system (Bilbao et al, 2021) which is used for the official WMO decadal forecasts. In the LANDMARC project, EC-Earth- CC, coupled to a land-use change model, is used to explore the feasibility and efficiency of LMT solutions (Land-based mitigation technologies).

The EC-Earth consortium is currently developing the next version of its Earth System Model, EC-Earth4. EC-Earth4 is based on OpenIFS and aims to incorporate the next major release 47R3 when available. EC-Earth4-CC, the carbon cycle version of EC-Earth4, will make use of the native tracer transport and advanced mass fixer schemes in OpenIFS, such as the updated Bermejo &

Conde fixer which is recommended for trace gases such as CO2. This will simplify model development and efficiency, compared to the EC-Earth3-CC model which relies on TM5. This ECMWF special computing project will pave the way for support of CO2 transport and treatment of various anthropogenic CO2 emissions sources in OpenIFS, through collaboration with the various research groups involved (ECMWF, WUR, KNMI, MPI, UU) and projects such as CoCO2 and the OpenIFS/CC space. It will also support the development of EC-Earth4-CC in support of large projects such as the recently granted Horizon Europe project OptimESM, involving a number of European modeling centers.

Subproject 2: CO_2 transport in OpenIFS and long-window data assimilation (WUR)

At Wageningen University, progress is being made on multi-tracer inverse modeling with CarbonTracker-Europe (CTE). Under the CoCO2 project we are now coordinating a study together with ECMWF on joint CO_2 and CO data assimilation that will focus on the 2019 Brazilian deforestation fires, using constraints from atmospheric samples and from TropOMI. An essential component of our inverse model is the atmospheric transport model TM5 (Krol et al., 2005), which is an offline model that simulates atmospheric transport using reanalysis meteorology fields from ECMWF.

We aim within this sub-project to first compare CO_2 transport between TM5 driven by the ERA5 reanalysis, and OpenIFS atmospheric transport nudged to ERA5. Recent progress at the Alfred Wegener Institute (Marylou Athanase) has facilitated the download, interpolation and use of ERA5 to nudge OpenIFS and we are planning to implement their method in EC-Earth4 with an interactive CO_2 tracer. A successful comparison and quantification of model-model transport differences is an important prerequisite for step 2: to repeat the CoCO2 study focusing on CO_2/CO assimilation windows with the OpenIFS model as transport operator.

Subproject 3: Multi-flux CO_2 transport in OpenIFS for hypothesis testing (MPI-BGC, UU)

The Max-Planck-Institute for Biogeochemistry (MPI-BGC, Jena) has a long history and experience in atmospheric transport modelling of CO2 surface fluxes. In the Jena Inversion System CarboScope, atmospheric CO2 transport is inverted so that the spatio-temporal distribution of CO2 sources and sinks can be inferred from atmospheric concentration measurements (e.g., Rödenbeck et al, 2003). These observation-based estimates have proven extremely useful in constraining the response of the climate carbon cycle system to increasing CO2 concentration simulated by Earth system models (e.g. Max-Plank Earth system model) – models which are used to project climatic changes throughout the 21st century (Winkler et al, 2019). A key part that remains unresolved, however, is the contributions of the various mechanisms that drive sinks and sources of CO2 at the land surface under increasing CO2 concentrations. In this subproject we aim to evaluate the different mechanisms represented in various flux products through atmospheric transport of spatially and temporally high-resolved idealized CO2 surface fluxes designed according to different mechanism hypotheses.

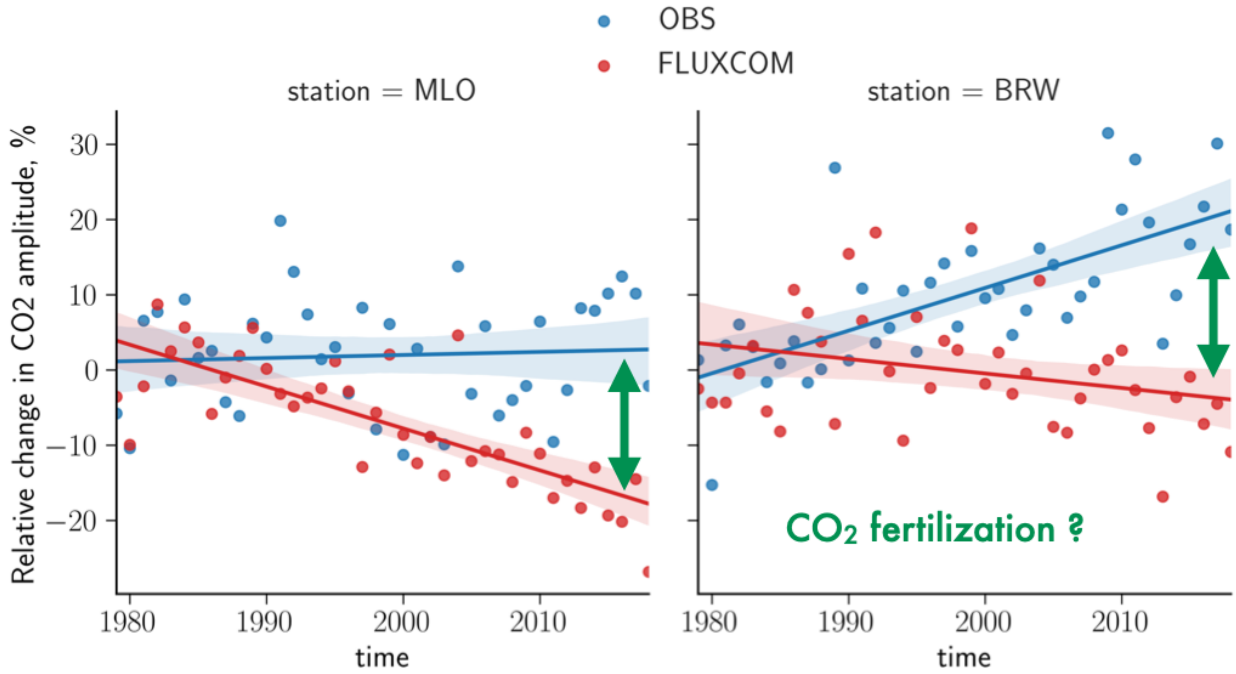

Figure 2 – **CO2 transport for hypothesis testing.** Divergence of observed and modelled seasonal cycle (amplitude) of atmospheric CO2 concentration. The transported CO2 land fluxes are estimated by the FLUXCOM project, which exclude the CO2 fertilization effect by design.

For instance, Figure 2 shows preliminary results from a modelling experiment using TM3, the core model in the CarboScope framework, that transports land-atmosphere CO2 surface fluxes estimated by the FLUXCOM project (including anthropogenic CO2 emissions, fire emissions and ocean fluxes). FLUXCOM is an initiative led by the MPI to upscale site-level measurements to global gridded estimates through machine-learning, using ERA5 reanalysis and remote sensing data as predictors. By design, this product excludes the CO2 fertilization effect as a key mechanism controlling the CO2 land sink. By comparing the transported idealized fluxes with atmospheric concentration measurements, we can estimate the contribution of each driving mechanism to the observed changes (e.g., here the effect of CO2 fertilization). Similar simulations have been performed, and are planned, for various ocean-atmosphere CO2 fluxes, for bottom-up derived CO2 fluxes (CMIP6 historical period), and for best-estimates derived from surface- and satellite datasets from, for example, the Global Carbon Project (GCP).

The main limitation of these transport models for described applications and research is its spatial resolution thus not explicitly accounting for essential transport processes such as convection. In collaboration with co-applicants from BSC, WUR, UU, and ECMWF, we aim to test OpenIFS as a transport model for high-resolution advection of idealized CO2 fluxes as a powerful tool to perform hypothesis testing regarding the mechanisms controlling land-atmosphere exchange of CO2. In accordance with Subproject 1 we first will focus on the low-resolution configuration of OpenIFS to develop and test atmospheric transport of CO2. In accordance with Subproject 2 we aim to explore the possibility to nudge the atmospheric transport in OpenIFS to the ERA5 meteorology to obtain high comparability between modelled and observed CO2 fluctuations. If the OpenIFS transport modelling tests are successful and promising, long-term forward runs in the high-resolution configuration

In addition to the above-mentioned, Utrecht University (UU, which recently signed the OpenIFS license and was already involved with EC-Earth) plans to perform forward simulations using the OpenIFS/CC model with biosphere fluxes from the data-based FLUXCOM product (Jung et al., 2020) and the process-based CTESSEL model. Besides the regular CO2 tracer, we will implement separate tracers to simulate the individual contributions of gross primary production (GPP) and terrestrial ecosystem respiration (TER) to the atmospheric CO2 signal. We will sample the tracers at station locations and compare to observations to assess model performance (e.g., increased seasonal amplitudes observed at Barrow that are ascribed to increased GPP, see Fig. 2). An additional aim is to simulate isotopic tracers of CO2 that can inform us on gross uptake by vegetation (e.g. δ18O, Δ17O and Δ47, Koren et al., 2019) or the water-use efficiency of the uptake (e.g. δ13C). Note that simulation of these isotopic tracers requires mass conservation, because small deviations in the mass of different isotopologues result in large variations in the isotopic signals.

In addition to the interest in the terrestrial exchange processes, UU has a specific focus on the carbon balance in tropical regions, which is also addressed in the recently funded TROPICS project. Although tropical regions dominate the interannual variability in the CO2 growth rate (Cox et al., 2013, Wang et al., 2013) the tropical regions are underrepresented from an observational and modelling perspective. We aim to explore variability in the CO2 fluxes from these regions, that is often related to drought or heat conditions, and assess its impact on atmospheric CO2.

Justification of resources

We ask for moderate computing and storage capacity, realizing that development of our codes and computing pipelines is not a highly computationally intensive task. Our main aim is to facilitate running the same codes, sharing input and output files, nudging data, and model configurations. We have chosen the Tco95L91 AMIP (OpenIFS dvien by observed ocean and sea-ice) configuration, at an estimated cost of 10k SBU/year, or 12.5k SBU/year when nudging is activated, as our main development configuration. This resolution is a compromise between resolution and wall-clock time that matches year-1 objectives and is also the main resolution chosen for EC-Earth4 development. We will also test the system at the Tl255L91 resolution (also at an estimated cost of 10k SBU/year), to compare results to previous modelling exercises done at this resolution, as well as a high-resolution configuration, such as Tco399L137 AMIP (in line with the simulations done in the CoCO2 project), with a cost estimated at 200k SBU/year for a limited number of years. Simulations planned will typically span several years to several decades, and only few ensemble runs are planned in this initial phase. Specifically, we plan:

In sub-project 1 (BSC): During the first year of this project (2023), we will work on developing and testing the updated version OpenIFS (47R3) using the low-resolution AMIP configuration of EC-Earth4, requiring 40 years of simulation. We will expand on the simulations done in 2022 with an earlier version of EC-Earth4 using OpenIFS 43R3v2. We will run two sets AMIP-style simulations from 1979-2019, one using the input4MIPS emissions and the other using the GridFED emissions, each one composing of a free running and another nudged to ERA5 (based on the developments done by WUR in sub-project 2) thus requiring 160 years. In total we will run 200 years which will cost approximately 2250k SBU (considering an average cost of 11.25kSBU/year). We will develop and test the high resolution (Tco399L137) configuration with free-running month-long tests and a few yearly-long tests (15 years in total, considering a cost of 200k SBU/year) using an estimated 2750k SBU, for a grand total of approx. 5000M SBU reserved for this sub-project. During the second year of the project (2024) we will repeat the low resolution runs using an updated and tuned version of EC-Earth4 (tuning will be done in another ECMWF special project spnltune) and will perform a large 40-year high resolution run for a total of approx. 10M SBU. Additional low-resolution members and longer high-resolution simulations will be performed on the Marenostrum4 and Marenostrum5 supercomputers. For data storage we require only 2TB to store input and output files.

In sub-project 2 (WUR): We plan up to ten runs at medium resolution (Tco95L91) nudged to ERA5 spanning 20 years (2M SBU), with four of those repeated at Tco399L137 (16M SBU). In addition we plan to run up to 30 short (~2 months) simulations at Tco399L137 resolution to create results comparable to the CoCO2 and CAMS IFS runs (1M SBU)). This leads to an expected usage of approx. 19 million SBUs over 2 years. We request disk space for the storage of the nudging files. The ERA-5 record spans 50 years, and the yearly files are approx. 2.5 GB/yr at T159 resolution. Together with other input data (fluxes, mole fraction data) that we want to keep archived with the simulations, we estimate the use of 6 TB of storage space. For further simulations we have access to national supercomputing facilities in Amsterdam, and in Bremen (Germany), on which OpenIFS has been set-up, compiled, and run already.

In sub-project 3 (MPI-BGC/UU): We aim to develop the model at low spatial resolution (Tco95L91) and conduct various (~60) short-term test-simulations (2-4 yrs) nudged to ERA5 for a total of 240 years and computational cost of 2700 kSBUs. Like in sub-project 2 we expect to conduct a limited amount of higher resolution (TCo399L137) runs with different sets of idealized surface fluxes (expected usage of 8000 kSBUs; 40 simulation years). We request disk space for the storage of test simulation output of 4TB. For further use of the developed OpenIFS/CC version we have access to the high-performance computing facilities at the German Climate Computing Center, Hamburg and computing and storage facilities offered through UU.

We require a total of 12 TB of tape storage, but would request a slightly larger value of 15TB to cover any unexpected needs.

Subproject	Simulated years Tco95 - 2022	Simulated years Tco399 - 2022	computational cost (kSBU) - 2022	Simulated years Tco95 - 2023	Simulated years Tco399 - 2023	computational cost (kSBU) - 2023
Subproject 1 (BSC)	200	14	**5050**	200	40	**10250**
Subproject 2 (WUR)	100	40	**9125**	100	45	**10125**
Subproject 3 (MPI-BGC / UU)	120	20	**5350**	120	20	**5350**
Total	420	74	**19525**	420	105	**25725**
Total w/ 10% buffer	462	81.4	**21477.5**	462	115.5	**28297.5**

Table 1 Summary of computational cost for each sub-project for both low and high resolution configurations

In total, our resources requested (detailed in Table 1), when considering a 10% buffer for retrial of failed runs will thus cover ~21M and ~29M in the first and second year, respectively, for a grand total of 50M SBUs on the ECMWF ATOS HPC. Requested storage adds up to 12 TB, but 15TB would allow for a modest margin covering unexpected needs.

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