REQUEST FOR A SPECIAL PROJECT 2022–2024

MEMBER STATE: …The Netherlands…………………………………………………...…

Principal Investigator[1]: …Prof. Dr. Wouter Peters………………………………………….……

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Other researchers: Gerbrand Koren (WUR), Alexander J. Winkler (MPI)

BSC: Etienne Tourigny, Iria Ayan

KNMI: Twan van Noije, Philippe le Sager, Vincent Huijnen

ECMWF: Glenn Carver, Marcus Koehler, Anna Agusti-Panareda, Gianpaolo Balsamo

Project Title:

OpenIFS Modeling of the Atmospheric Carbon Cycle (spoifscc)

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP** _________________	
Starting year: (A project can have a duration of up to 3 years, agreed at the beginning of the project.)	2022	
Would you accept support for 1 year only, if necessary?	**YES** ☐	

Computer resources required for 2022-2024: (To make changes to an existing project please submit an amended version of the original form.)	**2022**	**2023**	**2024**

High Performance Computing Facility	(SBU)	6M	0	0
Accumulated data storage (total archive volume)[2]	(GB)	15000	0	0

Continue overleaf

Principal Investigator: …Peters……………………………………

Project Title: OpenIFS Modeling of the Atmospheric Carbon Cycle (spoifscc)

Extended abstract

The carbon dioxide (CO_2) balance of the atmosphere is undergoing rapid change. While CO_2 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 CO_2 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 this carbon cycle hampers climate projections on decadal scales, but also complicates the attribution of observed CO_2 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.

Numerical modelling is key in climate predictions and in atmospheric CO_2 attribution, 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 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, and CoCO2 is strengthened by a large research community working with similar, or closely related, atmospheric transport models such as 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 CO_2) 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 future core of 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 new modelling capacity. This includes land-atmosphere feedbacks in the terrestrial biosphere, land-use change (LUC) scenarios that include short- (aerosol) and long-term (CO_2) climate impacts, and coupled carbon-water exchange for climate modelling. But also multi-tracer simulations, fast chemistry-schemes, ensemble predictions, and data assimilation (outside the scope of ECMWF's NWP setting) for enhanced MVS capacity. These applications all benefit when developed by a strong community focused on GHG modelling with OpenIFS:

(1) CO_2 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 to sacrifice 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 CO_2 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.

This proposal is a next step in the establishment of such a community, and the support of ECMWF in the form of a 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, Koren) and the Max-Planck-Institute for Biogeochemistry (MPI) in Jena, Germany (Winkler). These groups have been in close contact on the proposed development over the past 6 months, leading to the creation of the OpenIFS/CC (OpenIFS/CC : Carbon Cycle) group hosted in ECMWF at https://confluence.ecmwf.int/pages/viewpage.action?pageId=226496552, and plan to use the requested budget after divided equally over three different subprojects (i.e., ~2 million SBUs each). The sub-projects are described in more detail in the following sub-sections.

The three groups are supported by expertise from ECMWF (Carver, Koehler) and from KNMI in the Netherlands (van Noije, Huijnen, leSager). This takes the form of an advisory role for model-related questions and for technical challenges, but without a warranty of time from personnel to help the project succeed. Similarly, ECMWF greenhouse gas modelling experts (Agusti-Panareda, Balsamo) will provide advice and scientific feedback to the team but cannot commit to investing hours.

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

Subproject 1: CO_2 transport in coupled climate model with OpenIFS (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 CO_2, used in the emission-driven version of the model. The TM5 model is used for transport of CO_2 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 CO_2. 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 is working on the implementation of 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). Figure 1 shows results from the historical (concentration-driven) and esm-hist (emission-driven) historical experiments done for CMIP and C4MIP with the EC-Earth3-CC model. While the ocean-atmosphere fluxes are well simulated (panel d), very high CO_2 emissions coming from high from Land-use change (LUC) fluxes in the LPJ-GUESS model (compared to estimates from GCB2020, panel c) result in a high CO_2 bias (panel a) compared to observational record, which in turn lead to higher oceanic CO_2 uptake in the esm-hist simulation (panel d).

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. 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 CO_2. 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 CO_2 transport and treatment of various anthropogenic CO_2 emissions sources in OpenIFS, through collaboration with the various research groups involved (ECMWF, WUR, KNMI, MPI) and projects such as CoCO2 and the OpenIFS/CC space.

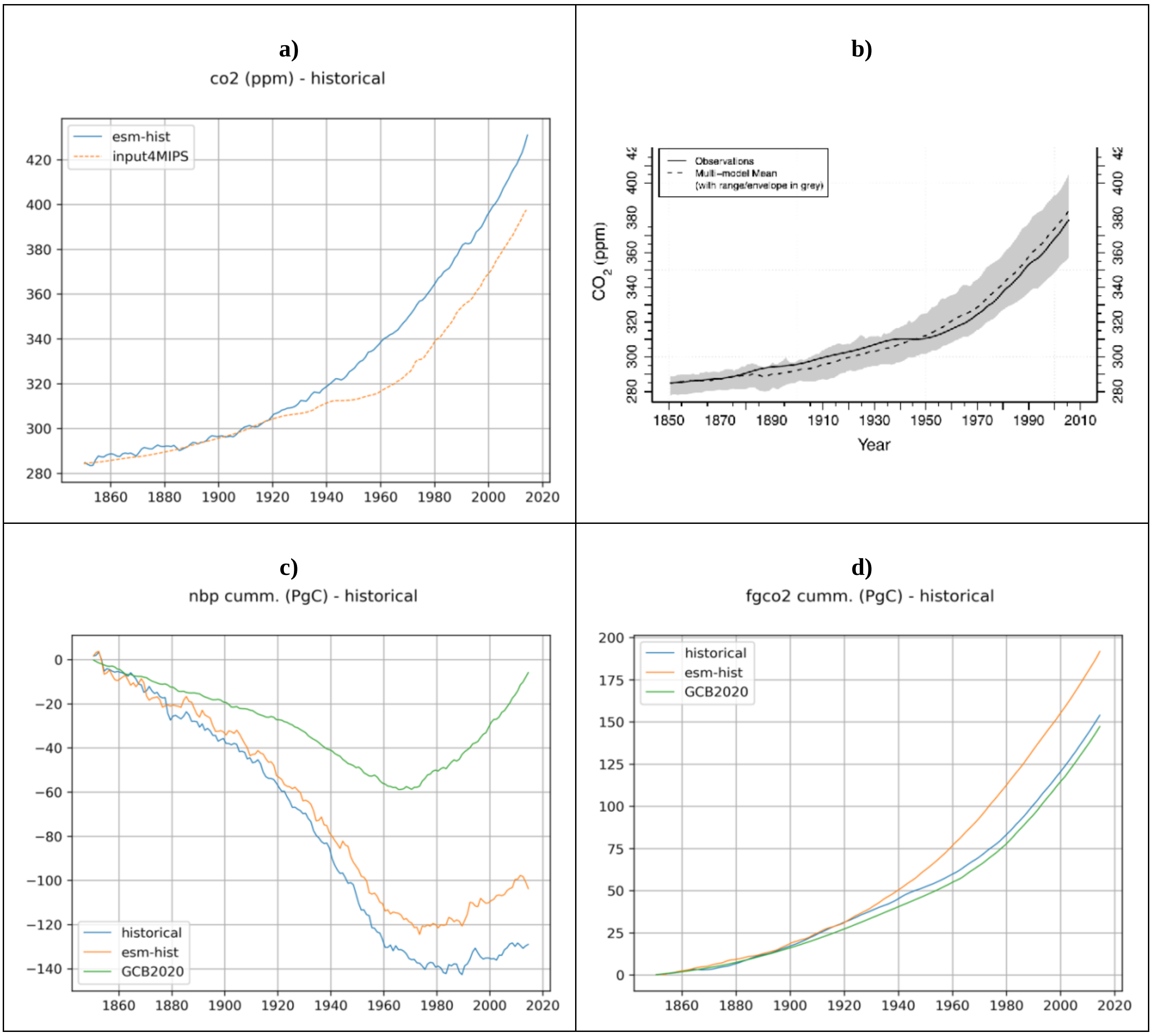

Figure 1 - results from the EC-Earth3-CC contribution to C4MIP historical and esm-hist

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

At Wageningen University, we have developed the CarbonTracker-Europe (CTE) inverse modelling system which is widely used to assess the carbon cycle. This includes studies on special events such as large-scale droughts (e.g., Wolf et al. 2016; Smith et al., 2020) and the yearly releases from the Global Carbon Project, (most recently by Friedlingstein et al., 2020). In addition, we have implemented multi-tracer versions of CTDAS such as the CO_2- δ13C system (van der Velde et al., 2018), and we are currently working on including more tracers (e.g., CO, N_2O), including our contribution to the CoCO2 project.

An essential component of the 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. The aim of this subproject is to work towards replacing the transport model TM5 with OpenIFS. The foreseen benefits include (1) being able to use a later version of OpenIFS than the dynamical core that was used to produce the reanalysis meteorology; and (2) avoiding the need of excessive data storage (~0.5 TB per year).

Using OpenIFS as a transport model in CarbonTracker-Europe will require some developments that also need to be tested. These modifications include the possibility to nudge the atmospheric transport in OpenIFS to be in agreement with ERA-5 meteorology. In addition, we need to include the possibility to set the initial CO_2 mole fraction fields from other simulations (e.g., from one of the CTE releases) and apply CO_2 emissions from fossil fuel combustion, biomass burning and the exchange with the biosphere and ocean. The modular design of the inverse modelling system CTDAS (van der Laan-Luijkx et al., 2017) allows a relatively easy transition to a new atmospheric transport model, such that the other components of the inverse model should remain unaffected.

Subproject 3: Multi-flux evaluations for CO_2 with OpenIFS (MPI)

The Max-Planck-Institute for Biogeochemistry (MPI-BGC, Jena) has a long history and experience in atmospheric transport modelling of CO_2 surface fluxes. In the Jena Inversion System CarboScope, atmospheric CO_2 transport is inverted so that the spatio-temporal distribution of CO_2 sources and sinks can be inferred from atmospheric concentration measurements (Rödenbeck et al, 2003). These observation-based estimates have proven extremely useful in constraining the response of the climate carbon cycle system to increasing CO_2 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 CO_2 at the land surface under increasing CO_2 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 CO_2 surface fluxes designed according to different mechanism hypotheses.

For instance, Figure 2 shows preliminary results from a modelling experiment using TM3, the core model in the CarboScope framework, that transports land-atmosphere CO_2 surface fluxes estimated by the FLUXCOM project (including anthropogenic CO_2 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 CO_2 fertilization effect as key mechanism controlling the CO_2 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 CO_2 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 in for example the Global Carbon Project (GCP).

The main limitation of the TM3 model in this application is its spatial resolution, which is limited to a grid of 4° latitude and 5° longitude (Heimann, 2003). In collaboration with co-applicants from BSC, WUR, KNMI, and ECMWF, we plan to test OpenIFS as a transport model for high-resolution advection of idealized CO_2 fluxes to perform hypothesis testing regarding the mechanisms controlling land-atmosphere exchange of CO_2. In concordance with Subproject 1 we first will focus on the low-resolution configuration of OpenIFS (Tco95) to develop and test atmospheric transport of CO_2. In concordance 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 CO_2 fluctuations. If the OpenIFS transport modelling tests are successful and promising, long-term forward runs in the high-resolution configuration and ensemble-mode will be conducted using the computing facilities at the German Climate Computing Center (DKRZ).

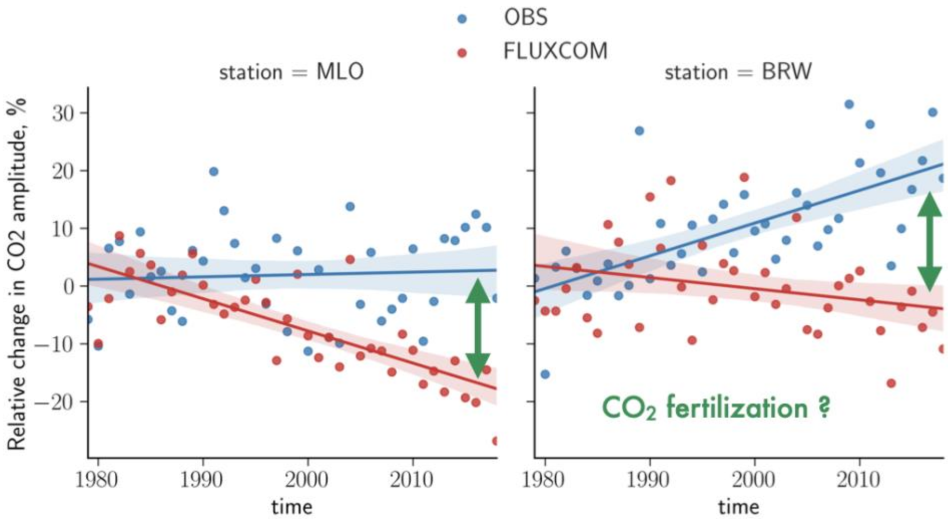

Figure 2 – Divergence of observed and modelled seasonal cycle (amplitude) of atmospheric CO_2 concentration. The transported CO_2 land fluxes are estimated by the FLUXCOM project, which exclude the CO_2 fertilization effect by design.

Justification of resources

In year-1 of our SP we ask for modest computing and storage capacity, realizing that development of our codes and computing pipelines is not necessarily a 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 Tco95L91 (at an estimated cost of 10k SBU/year, or 12.5k SBU/year when nudging is activated) as our main development vehicle, as a compromise between resolution and wall-clock time that matches year-1 objectives. We will also test the system at the Tl255 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 (in line with the simulations done in the CoCO2 project) 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: During the first year of this project (2022), the low-resolution configuration of EC-Earth4 which is Tco95L91 will be used to develop & test atmospheric transport of CO_2 in standalone OpenIFS and the ingestion of the input4MIPS historical SST and CO_2 emissions dataset used for the C4MIP exercise, with the land biogenic fluxes from CHTESSEL. We will run two AMIP-style simulations from 1979-2019, one free running and the other nudged to ERA5, for a total of 80 years. We estimate that 40 years of simulation will be required for development of the OpenIFS/CC model setup including support for CMIP6 emissions forcings and nudging, for a total of 120 years which will cost approximately 1350k SBU (considering an average cost of 11.25kSBU/year). We will perform short month-long tests in the high resolution (TCo399L137) configuration using the remaining 650k SBU of the 2M SBU reserved for this sub-project. Additional low-resolution members and longer high-resolution simulations will be performed on the Marenostrum4 supercomputer. For data storage we require only 2TB to store input and output files.

For sub-project 2: We plan up to six runs at relatively coarse resolution (Tco95) nudged to ERA5 spanning 20 years (1.5M SBU), in addition to a dozen short (~3 years) simulations at Tco95 and higher resolution (Tl255) for development/testing, leading to an expected usage of 2 million SBUs. 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.

For sub-project 3: We aim to develop the model at coarse resolution (Tco95) and conduct many (~30) short-term test-simulations (2-4 yrs) nudged to ERA5 for a total of 120 years and computational cost of 1500k SBU. Like in sub-project 2 we expect to conduct a limited amount of higher resolution (Tl255) runs with different sets of idealized surface fluxes (expected usage of 500 kSBUs). We request disk space for the storage of test simulation output of 2TB. 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.

Sub-project	Simulated years (Tco grid)	Cost in SBU (Tco grid)	Cost in SBU (other)	Total cost in SBU
Subproject 1 (BSC)	120	1350k	650k	2M
Subproject 2 (WUR)	120	1500k	500k	2M
Subproject 3 (MPI)	120	1500k	500k	2M

In total, our resources requested will thus cover ~360 years of lower resolution (Tco95) OpenIFS simulations for a total of 4.35M SBU and approximately 1.65M SBU at higher resolution, for a total of 6M SBU. We will perform initial testing on the TEMS HPCF, and switch to the ATOS HPCF once it is available, for the main production runs. Should the ATOS platform be delayed in production significantly, we will use the Cray XC40 (cca,ccb) platform with which we already have experience. Requested storage adds up to 10 TB, but 15TB would allow for a modest margin covering unexpected needs.

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