



Virtual Integration of Satellite and In-situ Observation Networks (VISION) v1.0: In-Situ Observations Simulator

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Abstract.

15 This work presents the first step in the development of the VISION toolkit, a set of python tools that allows for easy, efficient and more meaningful comparison between global atmospheric models and observational data. Whilst observational data and modelling capabilities are expanding in parallel, there are still barriers preventing these two data sources to be used in synergy. This arises from differences in spatial and temporal sampling between models and observational platforms: observational data from a research aircraft, for example, is sampled on specified flight trajectories at very high temporal resolution. Proper
20 comparison with model data requires generating, storing and handling a large amount of highly temporally resolved model files, resulting in a process which is data, labour, and time intensive. In this paper we focus on comparison between model data and in-situ observations (from aircrafts, ships, buoys, sondes etc.). A stand-alone code, In-Situ Observation simulator, or ISO_simulator in short, is described here: this software reads modelled variables and observational data files and outputs model data interpolated in space and time to match observations. This model data is then written to NetCDF files that can be efficiently
25 archived, due to their small sizes, and directly compared to observations. This method achieves a large reduction in the size of model data being produced for comparison with flight and other in-situ data. By interpolating global, gridded, hourly files onto observations locations, we reduce data output for a typical climate resolution run, from ~3 Gb per model variable per month to ~15 Mb per model variable per month (a 200 times reduction in data volume). The VISION toolkit is fast and easy to use, therefore enabling the exploitation of large observational datasets spanning decades, to be used for large scale model
30 evaluation. Although this code has been initially tested within the Unified Model (UM) framework, which is shared by the UK Earth System Model (UKESM), it was written as a flexible tool and it can be extended to work with other models.



1 Introduction

35 The importance of atmospheric observations from both in-situ and remote sensing platforms has been growing in the last few decades, with data archives, such as the new NERC Environmental Data Service (EDS¹), becoming a key infrastructure for the storage, exchange and exploitation of data. The strategic importance of in-situ measurements was also highlighted by the recent £49M NERC funding to maintain and re-equip the BAe-146 research aircraft of the FAAM Airborne Laboratory out to 2040.² Advances in geophysical model developments and exascale computing have similarly led to an increase in the complexity of models used for climate projections in international modelling projects, such as CMIP6; chemistry and aerosols components
40 are now routinely being included in a number of climate model simulations (Stevenson et al., 2020; Thornhill et al., 2021; Griffiths et al., 2021). Comparing all these models with observations is vital to increase our confidence in their ability to reproduce historical observations, understand existing biases and ultimately to improve their representation of the atmosphere.

A wide variety of observational datasets can be used for model evaluation; what makes such comparisons with model data
45 inherently difficult is the difference between the orderly model data (defined on a regular 3D grid and at regular time intervals) and the unstructured observational data (with variable coverage in space and time). A large computational effort is required for the handling and processing of gridded model data files into a format suitable for direct comparison with observations, especially when the measurement location varies with time (e.g aircraft, ships, sondes etc.). In order to compare to observational data with varying coordinates, model output must include hourly (or higher frequency) variables over a large
50 atmospheric domain. As well as being data-intensive, extracting hourly data from a tape archive is also time-intensive. This leads to orders of magnitude more data being stored, and processed than is actually required, and a significant amount of manpower and computer resources are spent to extract, read and interpolate model data in space and time onto desired observation coordinates. Because of these issues, previous studies of comparison between models and in-situ observations from aircrafts, are generally restricted to case studies over a limited number of campaigns (e.g. Kim et al., 2015; Anderson et
55 al., 2021), or compare model data with observed data independently of the time or location of measurement (e.g. Wang et al., 2020).

A previous attempt at producing Unified Model data on flight tracks was made several years ago, by embedding a `flight_track` routine (using Fortran programming language) within the UM-UKCA source code (Telford et al., 2013). However, using this
60 approach added a computational burden to the running of the UM-UKCA model and it was mainly intended for output of chemical fields (model diagnostics related to some UM dynamical fields were not available within the UM-UKCA subroutines). As a result, the `flight_track` routine used in Telford et al. (2013) was never ported to further versions of UM-UKCA.

¹ <https://eds.ukri.org>

² <https://www.faam.ac.uk/mid-life-upgrade/>



65 In this paper we describe the first tool in the VISION toolkit: `ISO_simulator.py`. This code can be embedded into the model workflow or can optionally be used as a stand-alone code with existing model data (e.g. to process variables from existing simulations). When `ISO_simulator` is embedded in the model workflow it produces much smaller data files which can be easily archived and are ready to be used for direct comparison with observations.

This new tool allows for routine production of model data interpolated at the time and location of in-situ observational data.

70 This can enable the exploitation of large observational datasets, potentially spanning decades, to be used for large scale model evaluation. The code is being developed to read any CF compliant model data and so could provide a valuable tool for supporting expanded diagnostics in upcoming CMIP7 experiments.

In section 2 we describe the `ISO_simulator` code, including command line arguments, input-output files and code optimisation. In section 3 we show how `ISO_simulator` is embedded within the Unified Model workflow. In section 4 we

75 provide some example plots showing comparisons of UM-UKESM modelled ozone to measurements from the Cape Verde Atmospheric Observatory (CVAO) (Carpenter et al., 2024), ozone measurements from the TOAR ocean surface database (including data from cruise ships and buoys, similar to Lelieveld et al., 2004 and Kanaya et al., 2019) and ozone measurements from the FAAM Airborne Laboratory (Smith et al., 2024).

2 Description of `ISO_simulator.py`

80 In order to run `ISO_simulator.py` the user will need access to python3.8 or higher, including CIS (Watson-Parris et al., 2016), `cf-python` (Hassell and Bartholomew, 2020) and Iris (Hattersley et al., 2023) APIs.

`ISO_simulator.py` performs the following steps:

1. Reads time and coordinates from observational files using CIS python libraries.
2. Reads all model variables from hourly files using `cf-python` libraries.
- 85 3. Co-locates model variables in space and time to the same time/location as the observations using CIS python libraries.
4. Writes monthly NetCDF files (Rew et al. 1989) containing model variables co-located onto flight tracks.

2.1 Input arguments

`ISO_simulator.py` requires a number of command line arguments which are shown in Table 1. The current version of

90 `ISO_simulator` was developed for use within the UM modelling framework and therefore some of the current command line arguments are UM specific. However, when interfacing `ISO_simulator` to different models, these command line arguments can be changed to reflect output data that is specific to each model.

A subparser argument, ‘`jobtype`’, is used to indicate whether the code is running within a model run-time workflow (if ‘`batch`’ is selected) or as a standalone postprocessing tool, e.g. on existing model data, (if ‘`postprocessing`’ is selected). These subparser

95 arguments also unlock specific conditional arguments: `--archive_hourly` can be used only if ‘`batch`’ is selected and `--`



select_stash can only be used if ‘postprocessing’ is selected. By default, when running in batch mode, all fields present in the output file being processed will be co-located to the observational locations.

ARGUMENT	DESCRIPTION
-i --inputdir <i>Directory_in</i>	<i>Directory_in</i> is the full path to the directory containing hourly pp files
-t --obsdir <i>Directory_obs</i>	<i>Directory_obs</i> is the full path to the directory containing observational files
-d --cycle_date <i>YearMonth</i>	<i>YearMonth</i> is a six digit tag to identify the start time of the analysis (YYYYMM)
-n --n_months <i>N</i>	<i>N</i> is the number of months to process, including <i>YearMonth</i> (optional; default 1)
-r --runid <i>UM_jobid</i>	<i>UM_jobid</i> is the unique identifier associated to a UM integration
-p --ppstream <i>Single_char</i>	<i>Single_char</i> is a single character identifying the hourly UM data ppstream as defined in Rose, e.g. k
-v --vertical_coord <i>coord</i>	<i>coord</i> is the coordinate for vertical interpolation: air_pressure or altitude; (optional; default=altitude)
-e --extra_file	<i>extra_file</i> is the filename (including full path) of model orography file; (optional, only required for hybrid theta-height coordinated if vertical_coord=altitude; default=Directory_ft/orography.pp)
-o --outdir <i>Directory_out</i>	<i>Directory_out</i> is the location to write output NetCDF files (optional). If <i>batch</i> is selected, output files are always written to <i>Directory_in</i> and additionally copied to <i>Directory_out</i> if present. If <i>postprocessing</i> is selected, output files are written to the current directory (./) or to <i>Directory_out</i> if present)
<i>batch</i>	Indicates the python script is running within the model workflow
-a --archive_hourly	<i>True</i> to keep model hourly files instead of deleting them (optional; default True)
<i>postprocessing</i>	Indicates the python script is running with existing model files
-s --select_stash <i>Code</i>	<i>Code</i> is a list of space separated UM stashcodes (an integer) to be interpolated (optional; default = interpolate all variables in the file)

100 **Table 1: Description of command line arguments used to run ISO_simulator.py**

2.2 Required Input files

Model input files can be supplied in NetCDF, UM pp and UM fieldsfile formats and must have a date tag in the filename (YYYYMMDD) to identify the date in the file. The ability to read different formats of model input files gives extra flexibility to the code as it allows to read other model data as well as UM data.

105 The interpolation code can use either air_pressure or altitude as the vertical coordinate for interpolation. If this is not specified it will use altitude by default. When using air_pressure as a vertical coordinate, model variables are output on selected pressure levels. Since the UM has a terrain following, hybrid height vertical coordinate system, we additionally need to output a Heaviside function that accounts for missing model data where a pressure level near the surface falls below the surface height



110 for that gridbox. Where data is valid, the Heaviside function has a value of 1, and a value of 0 otherwise. By dividing the model
field on pressure levels by this Heaviside function, the model data is correctly masked and missing data is assigned to invalid
gridpoints.

115 When using altitude as a vertical coordinate, because of the UM hybrid height coordinates, model variables are defined at
specified heights above the model surface; therefore, the model orography field has to be provided to correctly convert the
model hybrid height to altitude above sea level. The name and path of the orography file can be defined using the `-e` input
variable.

For observational data which is defined at the surface (ground measurements or ship/buoy data), a vertical coordinate is
generally not provided. In this case, `ISO_simulator` will use the model lowest level and interpolate in time, latitude and
longitude only.

120 As well as model files, input files containing information on the observational data coordinates are also required. These input
files should be in NetCDF format (Rew et al. 1989), all data should be organised in daily files, and each file must have a date
tag in the filename (YYYYMMDD) to identify the date of the measurement. As well as time and positional coordinates, an
optional string variable can be added to the observational input files to identify data belonging to a specific dataset or campaign;
this can help during analysis to subset relevant data, which is useful when comparing to several datasets/campaigns over a
number of decades. Existing observational data might require a degree of pre-processing to ensure files are in the right format
125 to be used by `ISO_simulator`; the extent and type of processing will vary depending on the format and structure of each
observational dataset.

2.3 Output files

130 The model data, co-located to the observational coordinates, is generated in NetCDF format files. `ISO_simulator` produces one
file per model variable per month. The size of these output files depends on the number and size of the observational files on
which the model data is co-located and therefore can vary each month.

2.4 Code Optimisation

135 There are several python libraries that can deal with reading and writing of large, gridded data files. The choice to use CIS
python libraries in `ISO_simulator.py` stems from their ability to handle ungridded data (such as data from ships, aircrafts etc.)
and the ease of performing co-location from gridded to ungridded data. However, initial tests showed that reading UM model
input files using CIS was significantly slower than reading the same file with Iris or cf-python; Table 2 shows reading times
for loading files in the following formats, UM fieldsfile, UM pp, and NetCDF, using different libraries. The tests were
performed on the JASMIN data analysis facility (Lawrence et al., 2012).

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N of fields in file	36	36	36	36	1	1
N of fields read	36	1	36	1	1	1
File format	UM fieldsfile	UM fieldsfile	UM pp file	UM pp file	UM pp file	Netcdf file
Field dimension	192,144,52,24	192,144,52,24	192,144,52,24	192,144,52,24	192,144,52,24	192,144,85,120
CIS	-	-	-	498.6 ± 7.1 s	16.5 ± 0.2 s	11.2 ± 0.1 s
Iris	229.1 ± 1.1 s	108.8 ± 1.0 s	255.5 ± 2.8 s	134.8 ± 1.7 s	6.8 ± 0.3 s	10.6 ± 0.1 s
Iris + structured UM loading	38.3 ± 0.8 s	39.6 ± 4 s	54.9 ± 3.8 s	52.9 ± 0.6 s	2.3 ± 0.3 s	10.4 ± 0.1 s
cf-python	12.8 ± 1.5 s	5.6 ± 2.3 s	14.0 ± 4.2 s	1.3 ± 0.2 s	2.6 ± 0.3 s	7.0 ± 0.1 s

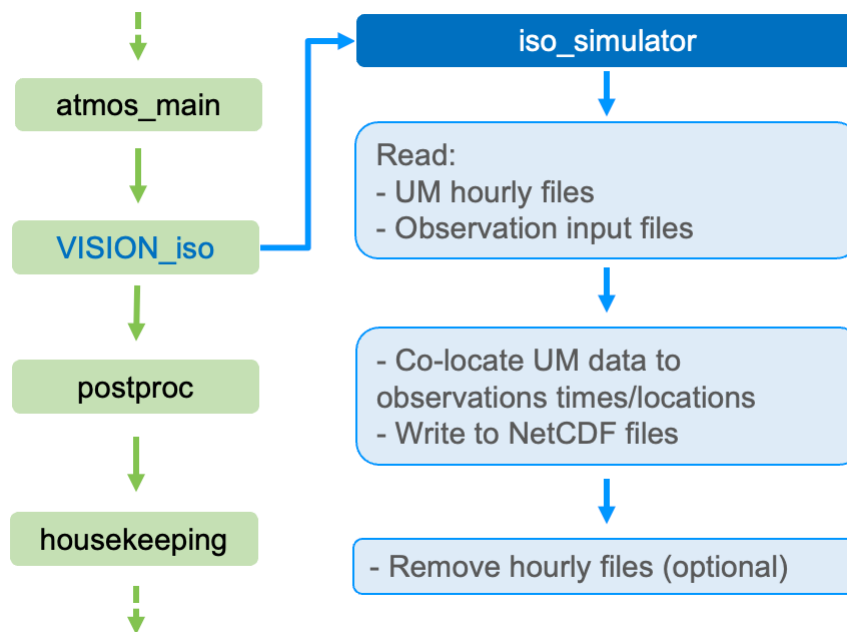
Table 2: Comparison of file reading times using CIS library (version: 1.7.4), Iris library (version: 3.1.0) and cf-python library (version: 3.13.0). The times in the table include reading the file and accessing the data numpy array (via a simple print statement) to avoid lazy loading. The numbers in the table are averages and standard error for reading each file several times on the JASMIN data analysis facility.

Given that potentially many such files would need to be read in each model month, cf-python was chosen to read the model data. However, CIS and cf-python use very different data structures for the gridded variables they read. In order to overcome this problem, a python function was developed to convert the cf-python gridded data structure to the CIS gridded data structure. Since reading model data is the slowest step in ISO_simulator, we further optimized the code by only reading model output files for days for which an observational input file exists.

3 Embedding ISO_simulator within the UM model workflow

This section describes how our code is interfaced within the UM framework. The UM uses Rose configuration editor (Shin et al., 2018) and the Cylc workflow engine (Oliver et al., 2018), respectively as a graphical user interface (GUI) and to control the model simulation workflow. Rose is a system for creating, editing, and running application configurations and it is used as the GUI for the UM to configure input namelists. Cylc is a workflow engine that is used to schedule the various tasks needed to run an instance of the UM in the correct sequence: for example *atmos_main* runs the main UM code, *postproc* deals with data formatting and archiving and *housekeeping* deletes unnecessary files from the user workspace.

A new Rose application, *VISION_iso*, was created and inserted into the Cylc workflow between the model integration step (*atmos_main*) and the *postproc* step (see Figure 1). This new application includes an input namelist and calls *ISO_simulator.py*; the NetCDF output files, containing model data co-located to the observations, are then sent to the MASS tape archive during the *postproc* step.



165 **Figure 1: A sketch of the UM run-time workflow, showing where the VISION toolkit is included.**

Since this software can be embedded into the UM run-time workflow and operates on UM output files (rather than being part of the UM source code), it has the following advantages compared to the approach in Telford et al. (2013):

1. Model data interpolated to the measurement times and locations is output using the internationally recognised NetCDF format, thus providing any required metadata information and making handling and analysis quicker and easier for users.
2. The code runs in parallel to the atmosphere model and does not affect the model run time.
3. The code can be easily customised to process any model data (not just UM data), therefore making it useful to the wider atmospheric science community.

175 Model data interpolated to the measurement times and locations can then be archived for long-term storage. When embedded into the UM workflow, data can either be transferred to the MASS tape archiving system or to the JASMIN data analysis facility (Lawrence et al., 2012). Further savings in data storage can be made by optionally deleting the hourly model output files used by the VISION toolkit.

4 Test Cases

180 In this section, we show some examples of using ISO_simulator to co-locate UKESM data to the same time and location as different types of observational datasets. Model simulations of UKESM were performed with a horizontal grid of $1.875^\circ \times 1.25^\circ$ and 85 vertical levels with a model top at 85 km and ERA reanalysis data was used to constrain the model



185 meteorology (Telford et al., 2008) to allow for better comparison with observations. For more information on the model configuration and details of the simulations, the reader is referred to the model description in Russo et al., (2023) and Archibald et al., (2024).

The aim of the plots in this section is not to answer specific science questions but to illustrate the way ISO_simulator can be used for comparison of model data with different sets of in-situ observations, namely: ground-based stations, ships/buoys, sondes/flights/UAV.

190 All model data is output hourly from UKESM, at a horizontal resolution of ~150km and then co-located, using ISO_simulator, to the same time and geographical coordinates as the observational data; the resulting data has the same time and spatial resolution as the observational data, making model data directly comparable to observational data. Furthermore, since the model and observational datasets can be compared over a long period of time, spanning several years, it is possible to sample seasonal and interannual variability, as well as better statistical sampling of extreme values. This type of comparison can greatly help to identify and improve model biases and to use models and observations in synergy to better understand
195 atmospheric processes.

4.1 Cape Verde Atmospheric Observatory

200 The Cape Verde Atmospheric Observatory (CVAO) provides long-term ground-based observations in the tropical North Atlantic Ocean region (16° 51' 49'' N, 24° 52' 02'' W). The CVAO is a World Meteorological Organisation-Global Atmospheric Watch (WMO-GAW) station; measurements from CVAO are available from the UK Centre for Environmental Data Analysis (CEDA) data archives (<http://catalogue.ceda.ac.uk/uuid/81693aad69409100b1b9a247b9ae75d5>, Carpenter et al., 2024). The University of York provides the CVAO trace gas measurements, supported by the Natural Environmental Research Council (NERC) through the National Centre for Atmospheric Science (NCAS) Atmospheric Measurement & Observation Facility (AMOF). Data from CVAO was chosen as an example of surface station data because the ozone
205 measurements are provided at a higher temporal resolution than the hourly model output; ISO_simulator can therefore be useful to interpolate model data in time to match the time of the observations.

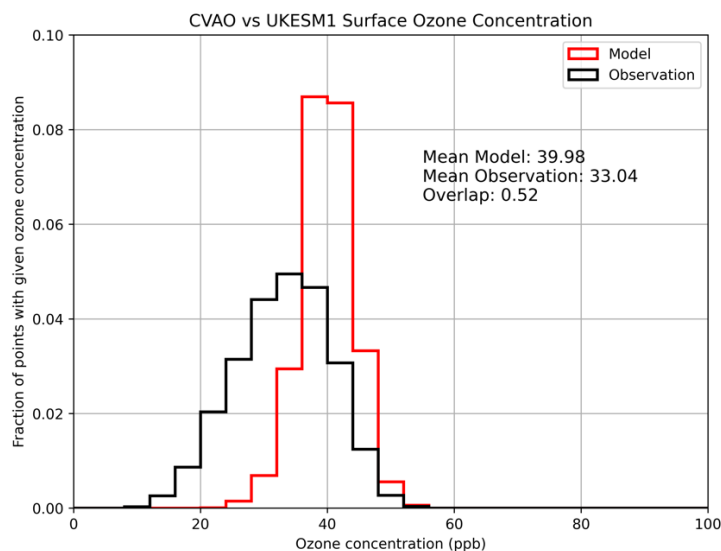


Figure 2: Probability distribution of ozone concentration at CVAO between 2007 and 2022. The black line shows observed ozone and the red line is model data co-located using ISO_simulator.

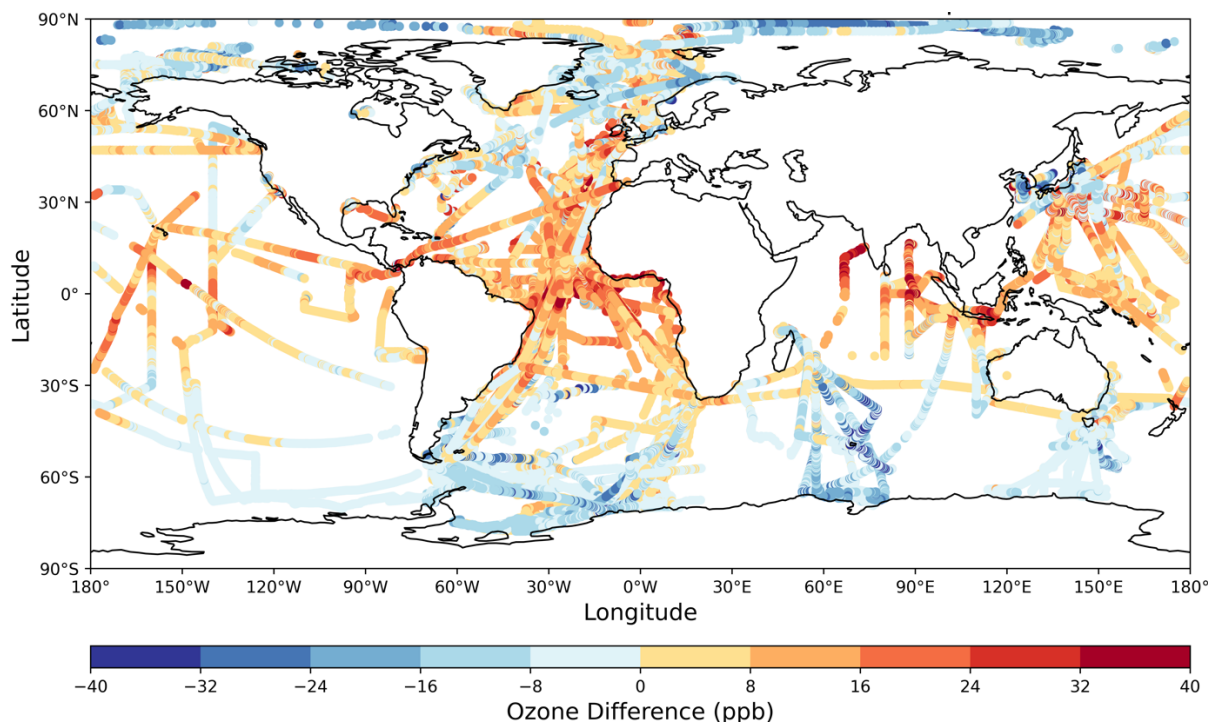
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4.2 Ships and buoys dataset

The Tropospheric Ozone Assessment Report (TOAR³) is an international activity under the International Global Atmospheric Chemistry project. It aims to assess the global distribution and trends of tropospheric ozone and to provide data that are useful for the analysis of ozone impacts on health, vegetation, and climate. A novel dataset has been produced by the TOAR “Ozone over the Oceans” working group. This dataset is an extension of previous similar datasets (Lelieveld et al., 2004, Kanaya et al., 2019) and it combines ship and buoys data from the 1970s to present day. This dataset will be released later this year as part of the TOAR-II assessment; given the large temporal span, this dataset constitutes a great example of using ISO_simulator to compare model and observational data over a large number of years.

UKESM data was co-located to the same times and locations as observations. The plot in Figure 3 shows the difference between modelled and observed ozone.

³ <https://igacproject.org/activities/TOAR/TOAR-II>



225 **Figure 3:** Map plot difference between UKESM ozone and observed ozone for the period Jan 1986 to May 2022. Model data is co-located using ISO_simulator.

4.3 Aircraft data: comparison to FAAM and ATom aircraft

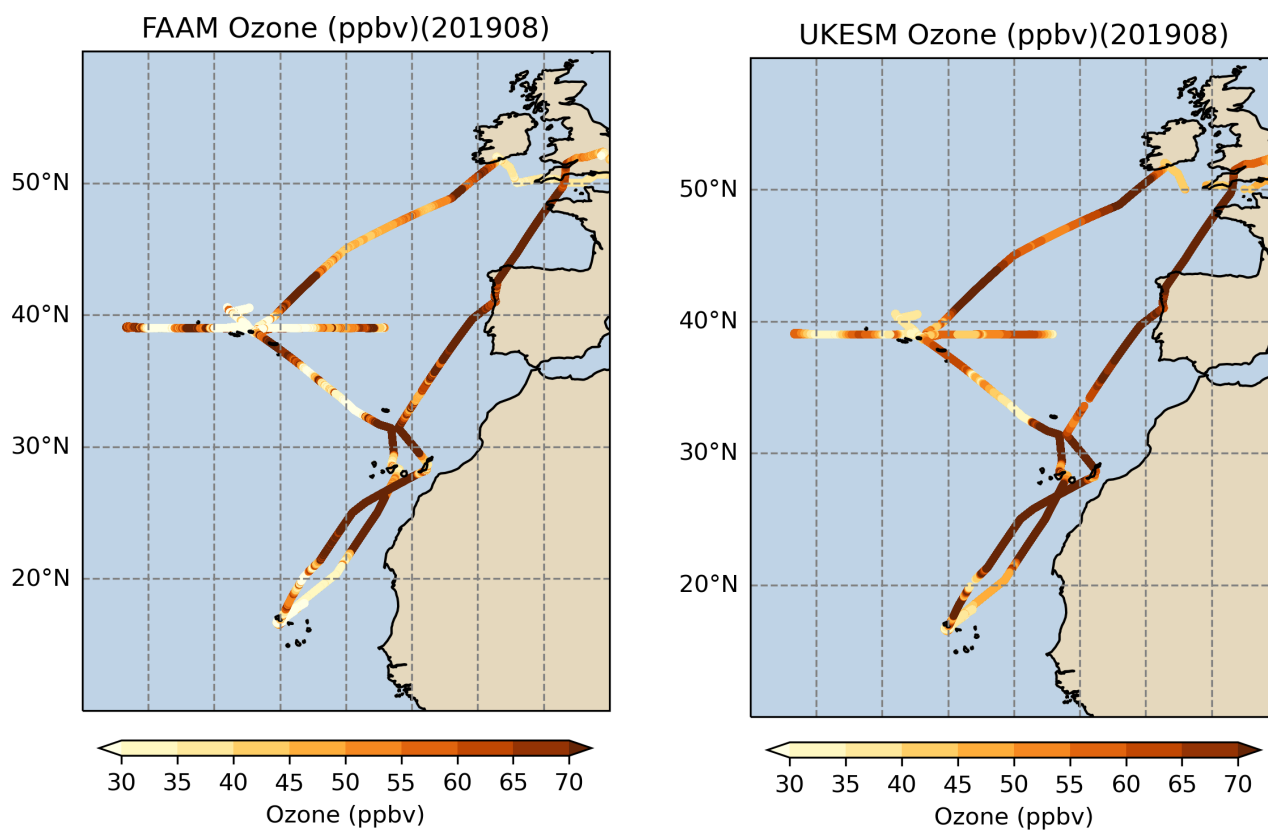
The FAAM Airborne Laboratory is a state of the art research facility dedicated to the advancement of atmospheric science. It operates a specially adapted, BAE-146-301 research aircraft, and is based at Cranfield University. The FAAM Airborne
230 Laboratory is funded by the Natural Environment Research Council and managed through the National Centre for Atmospheric Science (NCAS).

FAAM data from 2010 to 2020 was processed to extract ozone, time, latitude, longitude, air pressure and altitude and ensure variable names were consistent throughout this time period (Russo et al., 2024a). Figure 4 and 5 show comparison of modelled ozone and ozone observed by the FAAM aircraft. Figure 4 focuses on all individual flights from a specific campaign occurring
235 in Aug 2019. Figure 5 shows the difference between modelled and observed ozone for all flight points between the surface and ~ 6 km and for all FAAM flights between 2010 and 2020.

The NASA Atmospheric Tomography (ATom) mission was a global-scale airborne campaign, funded through the NASA Earth Venture Suborbital-2 (EVS-2) program to study the impact of human-produced air pollution on greenhouse gases and on chemically reactive gases in the atmosphere. ATom utilized the fully instrumented NASA DC-8 research aircraft to measure
240 a wide range of chemical and meteorological parameters in the remote troposphere (Thompson et al., 2022). Data from the ATom mission is available from the NASA data archive (<https://doi.org/10.3334/ORNLDAAAC/1925>, Wofsy et al., 2021).



Figure 6 shows ozone concentrations from ATom and UKESM, as a function of time and altitude, for a specific flight on the 3rd of February 2017.



245 Figure 4: FAAM and UKESM ozone concentrations (ppbv) for all flights in August 2019.

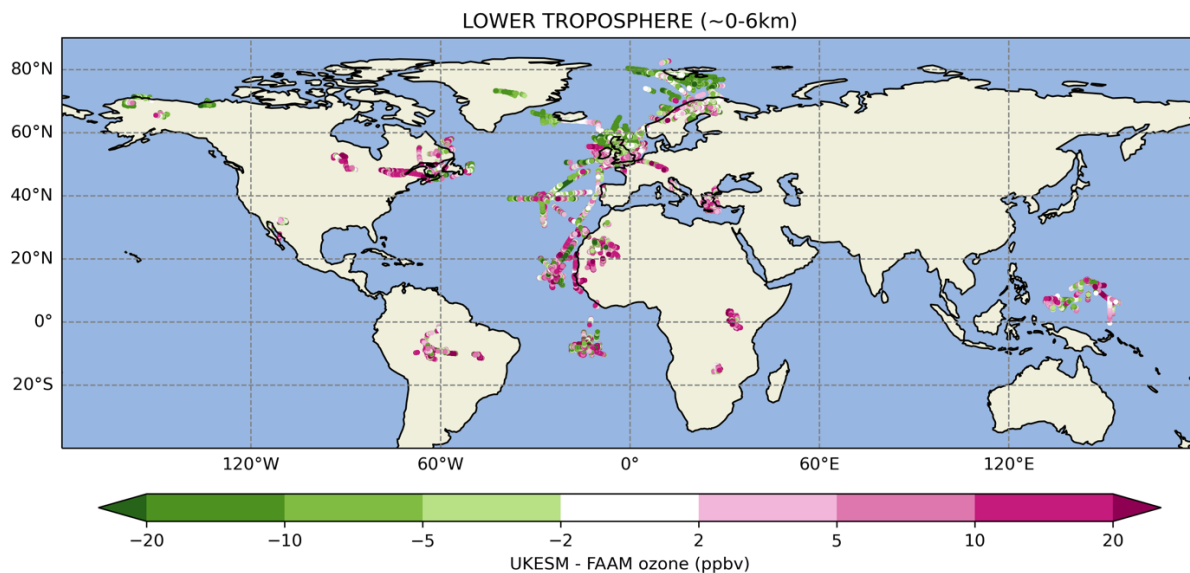
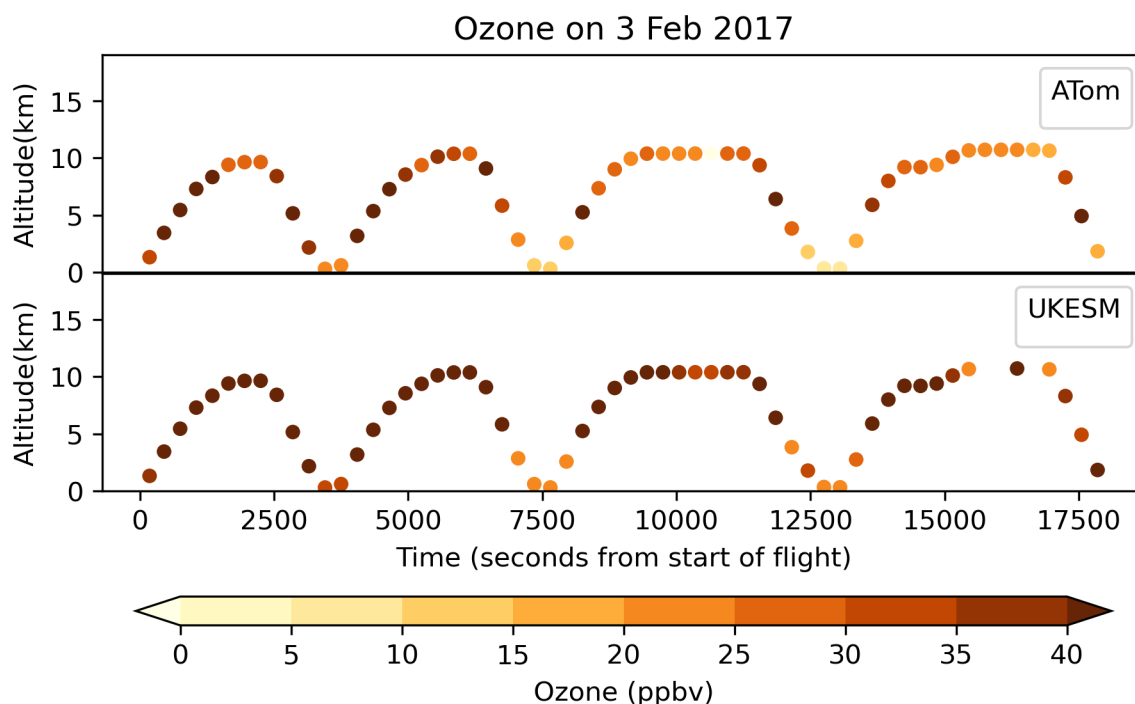


Figure 5: Difference between UKESM and FAAM ozone concentrations (ppbv) in the lower troposphere (0-6km) for all FAAM flights which measured ozone between 2010 and 2020.



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Figure 6: ATom and UKESM ozone concentrations (ppbv) for the ATom flight on 3rd of February 2017 from Hawaii to Fiji.



6 Conclusions

255 The ability to sample atmospheric model output at the same time and location as in-situ observations allows for better synergy between model and observational data, resulting in better understanding of atmospheric processes and more effective model evaluation. However, to do this usually requires the processing of large volumes of high frequency gridded model data. By interfacing with the CIS and cf-python libraries, we are able to efficiently automate this step, greatly reducing manual post-processing time and the volume of data that needs to be saved following a model simulation. This method is also transferable to many different atmospheric models, and the code is provided on GitHub under an open-source license.

260 The use of the cf-python library to read-in the UM-format files significantly decreases the time taken to read these files when compared to the Iris or CIS libraries. This further reduces the time required on the HPC batch system needed to post-process the files from the global model to the times and locations of the in-situ observations. An extension to this work is currently being carried out to be able to output model data on satellite swaths for better comparison between atmospheric models and satellite data.

265 Code and Data availability

The current version of the code presented in the manuscript is available on GitHub <https://github.com/NCAS-VISION/VISION-toolkit> and archived on zenodo (Russo et al., 2024b) <https://zenodo.org/records/10927302> under a BSD-3 license.

Input data are available from:

270 Modelled ozone (Abraham and Russo, last access Apr 2024),
<https://catalogue.ceda.ac.uk/uuid/300046500aeb4af080337ff86ae8e776>

FAAM ozone dataset (Russo et al., last access Apr 2024a),
<https://catalogue.ceda.ac.uk/uuid/8df2e81dbfc2499983aa87781fb3fd5a>

275 CVAO ozone dataset (Carpenter et al., last access Apr 2024)
<https://catalogue.ceda.ac.uk/uuid/81693aad69409100b1b9a247b9ae75d5>

ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols, Version 2 (Wofsy et al., last access June 2024),
<https://doi.org/10.3334/ORNLDAAC/1925>

Author Contribution

280 MRR developed the ISO_simulator code and processed the 11 year FAAM ozone dataset. MRR and NLA performed the UKESM model simulations. MRR, AMM and AJP performed data analysis and visualisation. NLA, EN, SLB, DH and DWP supported the development of the ISO_simulator code. DAS provided support with the FAAM data. NLA was the PI of the



projects leading to the development of ISO_simulator, supported by MRR, SLB and DH. MRR wrote the manuscript with contributions from all co-authors.

285 Competing Interests

The contact author has declared that none of the authors has any competing interests.

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