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AeroCom Aerosol GCM Trajectory Experiment

This document describes the AeroCom Air Parcel Trajectory experiment and the data we hope to obtain from modelling groups. The experiment aims to evaluate general circulation models (GCMs) against reanalysis meteorological fields combined with ground-based observations of aerosol properties in a trajectory-based Lagrangian framework to examine representation of source and transport dependence of aerosols to different regions globally.

The experiment only requests standard model output fields and should require no further model development. The experiment requests this standard output be in GRIB1 format. For three GCMs short post-processing scripts already exist to undertake post-processing of GCM output to GRIB1 format and these are available for two GCMs for direct use or adaptation. Instructions on how to locate these example scripts are provided at the end of this document.

Results will be published in peer-reviewed journals and all modellers that submitted data will be offered co-authorship. For any questions related to the guidance provided in this document please contact Daniel Partridge & Paul Kim using this Exeter University AeroCom mailbox (aerocom_trajectory@exeter.ac.uk).

Rationale

Aerosols are important components of the climate system; however, the impact of aerosols on climate remains highly uncertain due to the limited understanding of processes governing atmospheric aerosol sources and sinks. Historically, trajectory models have been used to study the role of transport in a Lagrangian framework and interpret source-receptor relationships and atmospheric processes for experimental data using meteorological fields from reanalysis data. However, GCMs provide the same output necessary for trajectory calculations to examine source and transport dependence of any simulated atmospheric constituent at any location for which we have corresponding observations.

Accordingly, applying trajectory calculations to the meteorological fields from reanalysis and GCM data for the same location and time-period (i.e. in a synchronised manner) facilitates a highly transparent means for evaluating the dependence of discrepancies between models and observations as a function of aerosol source/sink pathways during transport to a measurement station.

Trajectory analysis has been successfully applied to three GCMs that participated in the AeroCom Phase II Indirect 3 experiment (ECHAM6-HAM2; CAM5; HadGEM3-UKCA) to study how source-receptor relationships derived from simulated aerosol properties compare in the Arctic environment to observations from the Zeppelin station during 2001-2010 (Tunved et al., 2013; Partridge et al., in prep, 2017; P17 hereafter). Combining trajectory information with observed/simulated aerosol mass reveals large discrepancies between modelled and measured aerosol source functions. Whilst experimental data suggests major sources located in Russia/Siberia, model-derived results suggest major contributions arrive from Western Europe. The analysis technique will have wide scientific relevance as it facilitates tracing the aerosol evolution during transport to investigate the role of sources, dynamical processes and sinks on the aerosol properties in the model. By evaluating this information against observations, we will be able to pinpoint where, why and when the models underperform in their representation of aerosol properties.

In this AeroCom experiment we wish to extend the evaluation framework already established in P17 to a larger group of GCMs and measurement stations. Currently, a high number of measurement stations having long continuous measurements of aerosol properties exist from the EUSAAR measurement network; this experiment will tap into this invaluable resource to provide the wider aerosol modelling community with a better understanding of discrepancies between GCM simulated aerosol properties and observations to facilitate efficient model improvement. Trajectories will be calculated for the participating GCMs for a subset of ground-based measurement stations.

Questions to be explored

- 1.) Are the models capable of reproducing observed flow patterns in the atmosphere, and hence the role of aerosol emissions, processes and timescales? To understand if current GCMs can accurately represent aerosol transport it is of importance to understand how transport patterns compare to the reanalysis fields the models are nudged to.
    - To investigate this, GCMs will be run in nudged configuration and evaluated against ERA reanalysis products.
    - Resolution impacts on the representation of aerosol transport will be explored by using the new ERA-5 in this comparison at a range of resolutions, in addition to ERA-Interim for comparability with previous studies.
- 2.) How do the different models represent source-receptor relationships for simulated aerosol properties? How does this compare to experimentally derived source-receptor relationships?
    - For example, currently, there is no consensus on what sources and transport routes are responsible for transport of aerosols, especially absorbing material (BC) into the Arctic basin and there is an urgent need to better constrain the models.
    - By performing a trajectory pattern analysis or a potential source contribution function analysis (PSCF) will immediately reveal emissions hotspots influencing the receptor for which the trajectories are calculated. Furthermore, by comparing model derived emission hot spots and observationally derived hot spots one can directly identify weaknesses in the model representation of some certain key aerosol component.
    - Do the models reproduce the observed pronounced seasonal variation in Arctic aerosol number size distribution and related parameters such as integral mass and surface area?
    - By repeating this analysis for other stations experiencing different aerosol regimes (rural, continental, polluted) can we identify any regional/seasonal dependence in model-observation biases globally?
    - Can the GCMs represent the transport of aerosols from observed point source emission events, e.g. volcanic eruptions?
- 3.) What is the role of sink mechanisms for aerosols in the different models?
    - For example, are model-observation discrepancies in the simulated aerosol properties in the Arctic controlled by over(under)estimation of aerosol source regions or over(under)estimation of atmospheric sink processes such as wet deposition?
    - To investigate this, aerosol and meteorology data along the trajectories will be evaluated.

Tunved, P., Ström, J., and Krejci, R.: Arctic aerosol life cycle: linking aerosol size distributions observed between 2000 and 2010 with air mass transport and precipitation at Zeppelin station, Ny-Ålesund, Svalbard, Atmos. Chem. Phys., 13, 3643-3660.

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Experiment Description

Source-receptor evaluation of aerosol lifecycle in global climate models

The experimental design is now outlined. There are only two compulsory simulations for this AeroCom experiment. The first simulation is very short to allow for testing of model outputs prior to performing the core compulsory experiment.

IMPORTANT: To minimise resources, the first phase of this AeroCom experiment will only require submission of data pertaining to experiment ArcticTraj-DE. Accordingly, if you are performing your first simulations for the AeroCom Trajectory experiment only follow instructions related to this **development experiment** below. This will be used to assure conversion of all model output to the required format for trajectory calculations is correct before beginning the **core experiment**.

Experiments summary

1. **ArcticTraj-DE**: This is the compulsory development experiment. GCM Lagrangian evaluation of aerosol transport to the Arctic during summer 2006.
2. **Traj-NUDGE-CE**: This is the compulsory core experiment. GCM Lagrangian evaluation of aerosol transport to the ground based measurement stations (nudged simulations).

Development Experiment

1.) ArcticTraj-DE, compulsory

Evaluation of sources of aerosols to Zeppelin measurement station. A short 6-month simulation for one measurement station will be used to confirm post-processing for all participating GCMs is functioning correctly within the Lagrangian framework prior to the core experiment.

Simulation parameters:

- Simulation start 1st March 2006.
- Simulation duration: 6 months
- Spin-up: 3 months suggested (i.e. Dec 1st 2005: Feb 28th 2006)
- Historical Emissions (see references).
- Anthropogenic aerosol and precursor emissions: ACCMIP interpolated for the simulation years. With the upcoming production of simulation for the CMIP6 effort, many models should now have access to updated inventories. We recommend using the CMIP6 emissions if possible. (http://www.globalchange.umd.edu/ceds/ceds-cmip6-data/) for anthropogenic sources.
- Biomass-burning emissions: GFED3.1 for the simulation years.
- Greenhouse gas concentrations for year 2000.
- SST, sea ice: AMIP-style time-evolving.
- Ozone: RCP8.5.

Nudging:

Nudging horizontal winds (or vorticity and divergence) and pressure (but not temperature) towards ERA-Interim for the simulation years, using the default timescales for the model in question.

Model Complexity:

AMIP or PDRMIP style framework. Sea Surface temperature are prescribed. Aerosol direct, semi-direct, and indirect effects accounted for where available in the model.

Model Resolution:

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Global output is expected for standard model meteorological output variables (all diagnostics listed prior to aerosol diagnostics in provided spreadsheet). Model grid-box resolution is up to the modelling groups preference. For guidance, HadGEM3 is run at N96 resolution (1.25° in latitude by 1.875° in longitude).

Brief summary of required model diagnostics:

Aside from the standard meteorological variables in GRIB1 format needed for the trajectory calculations the aerosol analysis requires fields provided in NetCDF format. Details of the required model diagnostics to be provided can be found in the spreadsheet provided on the google drive.

Core Experiments

Core experiment: Traj-NUDGE-CE

Evaluation of sources of aerosols to global network of ground-based measurement stations having long-term continuous measurements of aerosol properties (see Appendix Table 1). We aim to include 10 measurement stations. At least one station will be selected from each region. This selection will be performed with the approval of participating groups AFTER the development experiment is complete. This core experiment will be used to answer key questions (1,2) (c.f. Rationale).

To answer key question 3 (c.f. Rationale) data from the GCMs along the trajectories is required. This necessitates high resolution output of aerosol fields globally to provide a much more rigorous evaluation of the GCM and facilitate untangling the contribution of aerosol sources/sinks to discrepancies between model and observations.

We understand that global 3D diagnostics will generate large data quantities. Accordingly, groups can choose to provide the requested aerosol diagnostics only at the station location for participation in key questions (1,2), however, please note that if data is provided at only the station location we will not be able to perform along trajectory analysis with your GCM.

Flexibility will be provided WRT simulation length if computing resources are an issue; in this instance the second half of the proposed time-period below can be used.

Simulation parameters:

As in experiment Arctic_Traj-DE with the following additions:

Time period: 1 Jan 2000 to 31st December 2010 inclusive. These dates might get adjusted after selection of participating measurement stations to ensure optimal measurement data coverage.

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Global Meteorological Model Output Diagnostics, GRIB1 format

File format and structure: GRIB1

- Fields in this format are required for subsequent trajectory calculations (to be performed by University of Exeter). These fields correspond to those labelled BOTH in the provided spreadsheet.
- When running the ArcticTraj-DE development simulation, we also require the diagnostics in NetCDF format to allow for any troubleshooting of potential problems in the trajectory calculations. This duplication will NOT be required for the core experiment.
- This data to be uploaded at University of Exeter server, instructions at end of document.
- Format should conform to example GRIB1 files (location provided at end of document).
- Important: When providing fields associated with GRIB format all fields should be within one single GRIB file for each month.

Filename convention:

trajectory_aerocom_<ModelName>_<ExperimentName>_ <month>_<year>_<Frequency>.grib

for ArcticTraj-DE also provide same diagnostics in NetCDF format using same convention:

trajectory_aerocom_<ModelName>_<ExperimentName>_ <month>_<year>_<Frequency>.nc

- <ExperimentName> should be one of these options:

- ArcticTraj-DE
- Traj-NUDGE-CE

All fields should be provided instantaneously at 3-hourly resolution (except surface fluxes, see spreadsheet).

Example GRIB1 files for ECHAM-HAM and CAM will be made available, as well as required post-processing scripts to convert standard output into the required GRIB1 format for these models.

The University of Exeter will be responsible for archiving the trajectory fields calculated from these GRIB1 files in NetCDF format at the AEROCOM server.

Note: The trajectory software uses the GRIB centre code to determine what tables to assume and so which parameters to use. It currently understands ECMWF (98), UKMO (74), and NOAA NCEP (7) or other centers running NCEP models (AR, 42 and FNMOC, 58). For models which can output GRIB natively using a different centre code please contact us prior to proceeding; if converting from another format it's probably best just to use the ECMWF tables in most cases.

2D fields: Instantaneous, 3-hourly resolution

The precipitation and surface sensible heat flux should be time-integrated, i.e. if they're output as per-unit-time fluxes they should be multiplied by the time interval of the data.

Model Specific Notes:

ECHAM: As this model has been used successfully we have already applied the necessary conversion factors for precipitation/relative humidity in our subsequent trajectory framework (detected by its use of the GRIB sub-centre field). Therefore, for this model we can process the GRIB output obtained using the provided example scripts directly.

3D fields: Instantaneous, 3-hourly resolution

3D fields should be on either hybrid sigma-pressure model levels (correctly described in the GRIB file), or interpolated if necessary onto fixed pressure levels. Hybrid-height model levels and fixed height levels are untested currently. If your model uses hybrid-height model levels please let us know before starting any simulations.

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Aerosol and related Fields in NetCDF format for evaluation against measurement stations/along trajectories

File format and structure: NetCDF. Corresponds to diagnostics labelled NetCDF in spreadsheet provided.

- Fields in this format are required for linking station observations to trajectories.
- NetCDF Data should be uploaded to the University of Exeter server. The University of Exeter will subsequently upload these files to the AeroCom server at the same time as uploading the trajectory files in NetCDF format after converting from the GRIB1 files provided by participating modelling centres. .
- One NetCDF file per year of data.

Filename convention:

trajectory_aerocom_<ModelName>_<ExperimentName>_<VariableName>_
<month>_<year>_<Frequency>_<{Station/Global}>.nc

All 2D data have dimension (lon x lat x time x {station if plan to participate in key questions 1,2 only}).

All 3D data have dimension (lon x lat x level x time x {station if plan to participate in key questions 1,2 only}).

- <VariableName> correspond to the variable short_name (see spreadsheet provided).

<{Station/Global}> correspond to participation in key questions. If participation only in key questions 1,2 please label <Station>. If participation in all key questions, please label <Global>.

- <ExperimentName> should be one of these options:

- ArcticTraj-DE
- Traj-NUDGE-CE

Aerosol fields: 3D, Instantaneous, 3-hourly resolution

We will require diagnostics for all the per-mode/component number and mass tracers plus dry and wet radii diagnostics, "or the nearest equivalent" for models which are formulated differently. Any metadata required to interpret these should be provided as standardised attributes on the relevant tracers (e.g. one for number fields for the geometric standard deviation of the mode).

For the M7-style modal models (HAM, GLOMAP etc), a standard convention for presenting the number and mass tracers along with metadata for mode width parameters etc. can be specified. However, due to the nature of different aerosol schemes different GCMs will have a different set of components (e.g. nitrate, ammonium, separate SOA etc.) and possibly a different number of modes (e.g. MAM3).

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Data Upload

Post-processing of the model data into trajectories requires specialised software and significant computing resources (storage/processors). Accordingly, to reduce the computer/human time input of participating modelling centres we have setup a post-processing server hosted at the University of Exeter to calculate the GCM trajectories for each model and convert these into CF compliant NetCDF files for final upload to the AEROCOM server. Below are instructions for uploading the data to this server for the development experiment located in a folder called ArcticTraj-DE on your server:

rsync -av ArcticTraj-DE exeter_aerocom@stratus.ex.ac.uk::centrename/aerocom_trajectory

The following username and password should be used to connect to this server space for data upload. Please do not distribute this password to anyone else and be careful to only upload data to your own centrename.

username: exeter_aerocom

password: vk8gxzGc

Each group has been allocated their own unique centrename to be used in the command above (replace the text centrename with the name allocated to your group).. Your centrename can be found on the provided spreadsheet. This can be found on this google drive link (for which you do not need a google account)::

https://drive.google.com/drive/folders/1CKbWRN1-7zjn6TaaZQHDS0Veo4FHO8d2?usp=sharing

Please do not distribute this link to anyone else.

This link will give you access to an AeroCom folder which contains the centrename spreadsheet as well as a copy of this document and other important files (diagnostic spreadsheet and example scripts). When you open the spreadsheet to find your centrename please also check the other information provided for you and the blank columns where we require information for each of your models for publications arising from this experiment. The centrename spreadsheet is editable directly so please complete/update the sections of this document relevant to your group directly using google docs.

Example data and processing scripts

IMPORTANT: We have provided example GRIB1 files for the meteorological variables that we know work with the trajectory software for both ECHAM-HAM and CAM. These example files along with post-processing scripts used to generate them and a README file can be found at this location on our Exeter servers: exeter_aerocom@stratus.ex.ac.uk::examples and can be accessed using the above username/password.

They will also be provided on the google drive link above for convenience.

Please refer to these files and scripts as reference points when generating your GRIB1 files for submission. One tool that can be used to inspect your GRIB files for comparison is Meteoinfo which can be downloaded here:

http://www.meteothinker.com/downloads/index.html

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References

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Anthropogenic emissions: ACCMIP/MACCity

http://ether.ipsl.jussieu.fr/eccad

Granier, C. et al.: Evolution of anthropogenic and biomass burning emissions of air pollutants at global and regional scales during the 1980–2010 period, 2011.

Diehl, T.: Anthropogenic, biomass burning, and volcanic emissions of black carbon, organic carbon, and SO2 from 1980 to 2010 for hindcast model experiments., doi:10.5194/acpd-12-24895-2012, Atmospheric Chemistry and Physics Discussion 12: 24895-24954, 2012.

Lamarque, J.-F.: Historical (1850–2000) gridded anthropogenic and biomass burning emissions of reactive gases and aerosols: methodology and application, doi:10.5194/acp-10-7017-2010, Atmospheric Chemistry and Physics 10: 7017-7039, 2010.

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Appendix Table 1 (10 station sub-selection with participating groups after development experiment completed)

	Station Code	Station	Lattitude (Decimal)	Longitude (Decimal)	Height m.a.s.l
Station Index	Low altitude sities (< 1000 m.a.s.l)				
	Arctic				
1	ZEP	Zeppelin	78.906	11.888	474
2	NRD	Station Nord	81.600	-16.670	30
3	ALT	Alert	82.500	-62.300	210
4	BRW	Barrow	71.320	-156.616	8
5	TIK	Tiksi	71.600	128.890	35
	Nordic & Baltic				
6	ASP	Aspvreten	58.800	17.383	30
7	BIR	Birkenes	58.383	8.250	190
8	PAL	Pallas	67.967	24.117	560
9	PLA	Preila	55.370	21.030	5
10	SMR	Hyytiala (SMEAR II)	61.850	24.283	181
11	VHL	Vavihill	56.017	13.150	172
12	TTU	Tartu	58.370	26.740	40
13	VIL	Vilnius	54.643	25.183	170
14	VRO	Värriö	67.767	29.583	400
	Central Europe				
15	BOS	Bosel	53.000	7.950	16
16	KPO	K-Puszta	46.967	19.317	125
17	MPZ	Melptiz	51.540	12.930	86
18	OBK	Kosetice	49.580	15.250	534
19	HPB	Hohenpeissenberg	47.800	11.010	986
20	WAL	Waldhof	52.800	10.756	75
21	PRG	Prague	50.127	14.385	190
	Western Europe				
22	CBW	Cabauw	51.971	4.927	1
23	HWL	Harwell	51.567	-1.317	60
24	NKEN	North Kensignton	51.521	-0.214	5
25	MHD	Mace Head	53.326	-9.904	5
26	LYN	Lyon	45.779	4.882	185
27	MDR	Madrid	40.456	-3.730	669
28	PAR	Paris (SITRA)	48.718	2.207	156
	Mediterranean				
29	FKL	Finokalia	35.330	25.670	250
30	IPR	JRC-Ispra	45.820	8.630	209
31	CAP	Cap Corse (CHARMEX Supersite)	42.969	9.380	516
32	MNY	Montseny	41.779	2.358	720
33	NEO	Navarino Observatory	36.830	21.704	53
	Misc.				
34	ASI	Ascension Island (ARM)	-7.970	-14.405	76
35	MCO	Maarco, UAE (Arabian Gulf)	24.700	54.659	5
36	GRA	Granada	37.164	-3.605	680
37	OPE	Observatoire Perenne de l'Environnement	48.562	5.506	392
38	ABU	Annaberg-Buchholz	50.572	12.999	545
39	NGW	Neuglobsow	53.167	13.033	62
40	LMO	L.mesto	50.661	14.040	147
41	VLM	Vielsalm	50.304	6.001	496
42	ATH	Athens	37.991	23.810	270
43	LEC	LecceECO	40.336	18.125	36
44	GIO	GiordanLighthouse	36.072	14.218	167
45	AYO	Anmyeondo, South Korea	36.538	126.330	46
46	DRE	DresdenWinckelmannstrasse	51.036	13.731	120
47	NMY	Neumayer	-70.666	-8.266	42
48	GPA	GualPahari	28.428	77.151	320
49	WVB	Walvis Bay (Airport)	-22.980	14.374	n/a
50	STH	St Helena	-15.942	-5.667	435
51	GOB	Gobabeb	-23.562	15.041	405
52	HEN	Henties Bay	-22.095	14.260	20
53	NAN	Nanjing (SORPES)	32.121	118.953	40
54	BAL	Balia	25.800	84.200	64
55	GUW	Guwahati	26.183	91.733	55

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Appendix Table 1 continued:

	Station Code	Station	Lattitude (Decimal)	Longitude (Decimal)	Height m.a.s.l
	High altitude sities (> 1000 m.a.s.l)				
	Western Europe				
56	PDD	Puy de Dôme	45.772	2.966	1465
	Central Europe				
57	SSL	Schauinsland	47.917	7.917	1210
58	ZSF	Zugspitze	47.417	10.983	2670
59	JFJ	Jungfraujoch	46.548	7.985	3571
	Balkans				
60	BEO	Moussala	42.180	23.585	2925
	Mediterranean				
61	CMN	Monte Cimone	44.200	10.700	2165
	North Pacific				
62	MLO	Mauna Loa Observatory	19.540	-155.580	3397
	Nordic & Baltic				
63	ARE	Åre	63.427	13.077	1242
	Misc.				
64	SMT	Summit	72.596	-38.422	3209
65	PIC	PicduMidi	42.937	0.142	2877
66	IZA	Izana	28.309	-16.499	2373
67	NEP	NepalClimateObservatoryPyramid	27.958	86.815	5079
68	CHAC	Mount Chacaltaya	-16.350	-68.131	5320
69	TRO	Trollhaugen	-72.012	2.535	1553