A OFFLINE TRAJECTORY PACKAGE (version 3) Where to Find the Package and How to Use It

The "Offline" trajectory package can currently be found on the computer fuji provided by the CSAR service at Manchester.

Example jobdecks	/home/fuji/lrjm4/outside/offline_3/siua.job
	/home/fuji/lrjm4/outside/offline_3/llpr.job
	/home/fuji/lrjm4/outside/offline_3/umtraj.job
Source code listing	/home/fuji/lrjm4/outside/offline_3/offline_3.src
Updates directory	/home/fuji/lrjm4/outside/offline_3/updates
Programme library	/home/fuji/lrjm4/outside/offline_3/offpl

The following libraries are also used when reading wind data:–

ECMWF records	:	/home/fuji/lrkd/lib/libemosR8.a
UKMO UM PP-files	:	/home/fuji/lrkd/lib/libffio32.a
UKMO UM PP-files	:	/home/fuji/lrkd/lib/libumgrib32.a
UKMO UM PP-files	:	/home/fuji/lrkd/lrrb3/umdiagn/libsumo12.a

The example jobdeck "siua.job" calculates 0.5 day back trajectories from 2001073112 to 2001073100 (meaning YYYYMMDDHH). The particles are initially (at 2001073112) grouped into 2 clusters on the 900 hPa and 800 hPa surfaces. The data containing the winds is found in the ECMWF, upper air, initialised, spectral analyses:–

siua2001073112, siua2001073106, siua2001073100.

If specific humidity is required as an attribute the files giua2001073112... (containing q on an N80 grid) are also needed.

The example jobdeck "llpr.job" performs a similar trajectory calculation but using $2.5^\circ \times 2.5^\circ$ gridded analyses (llpr82120112...). Importantly these low resolution analyses are on pressure levels and prescribed ω_L is used for vertical velocity (rather than η and calculated $\dot{\eta}_{L+\frac{1}{2}}$). Since surface pressure is not contained in these records an appropriate surface orography file (e.g. lior89010100) must be provided in order to check that particles do not stray below ground.

The first calculation using the much higher (horizontal and vertical) resolution spectral analyses (siua2001073112...) is more accurate than the second calculation using the gridded, pressure level analyses. However, the memory and CPU requirement is significantly higher

(CPU is 8 times higher for the above example). If high accuracy is required then the spectral analyses have the advantage of being more compact and allow the calculation of $\dot{\eta}_{L+\frac{1}{2}}$ which leads to a great improvement in advection close to the ground. In addition, potential vorticity and any other dynamical fields can be derived from the spectral analyses.

Information on the content of ECMWF analyses, file-naming and access to the data itself can be found on the World Wide Web site run by the BADC (*http://www.badc.rl.ac.uk/*).

The example jobdeck "umtraj.job" calculates similar 5 day back trajectories using UKMO Unified Model data, from 28090606 to 28090106, at climate resolution. In this example the input data is expected in the files:–

ccmfna.pam8966.pp, ccmfna.pam8960.pp, ..., ccmfna.pam8916.pp .

Since potential temperature is specified as a trajectory attribute, the data files are expected to contain temperature or potential temperature in addition to winds and surface pressure.

B Parameters and Namelist Controls

There are fourteen fundamental parameters which are required for the operation of Offline (listed in Table 1). NN → NTRAC describe the sizes of the fields containing spectral and grid point winds and attributes. For T106 ECMWF analyses ("siua" files) the recommended values for MG and JG are given as default. These correspond to the quadratic Gaussian grid (N80) at T106 resolution which is also appropriate for the specific humidity field archived in "giua" files. When using $2.5° \times 2.5°$ data ("llpr" files) you should use MG=144 and JG=35 (the number of latitudes in one hemisphere, not including the pole and equator). For UKMO Unified Model data at the current climate resolution you should use MG=96 and JG=36. NPART, IPTS, NATTR and MAXCLUS specify the sizes of arrays associated with the trajectories themselves. The input and output channels used by Offline are detailed in Table 2.

The operation of Offline is controlled by the namelist variables. Namelist INPNAME (Tables 3 and 4) specifies the format and contents of the wind records and the timing operation. In addition, selected fields can be assigned as particle attributes. The basic time-stepping between wind records is controlled by BEGDAY, THIST, LFORW and the parameter IPTS. The number of time-steps used by the trajectory integration between consecutive wind records is given by NSTEPS and the frequency that trajectories are recorded and output is controlled by LEVERY and NSKIP. The length of each trajectory (T, in days) is calculated from IPTS, THIST and NSTEPS (see Table 4).

Most effort in the trajectory calculation is often expended in retrieving the winds and attribute fields (especially if spectral transforms are required). If many sets of trajectories with staggered release times are required then greater efficiency is achieved by integrating the co-existing trajectory sets in parallel using the "multiple" set feature. In this case *sets* of trajectories are released at interval TRELEASE, the length of each trajectory (T) is determined by IPTS (as in Table 4), and the total length for the calculation of all sets is controlled using TINTEG.

For example, you would like to calculate sets of 5 day back trajectories to be released at daily intervals throughout a whole month, given wind analyses at 6 hourly intervals. The required namelist settings would be:

```
BEGDAY=0., THIST=0.25, LFORW=.FALSE., LEVERY=.FALSE., IPTS=21,
LMULTI=.TRUE., TRELEASE=1., TINTEG=35.
```

Note that TINTEG includes 31 release dates (i.e. 2001073112 → 2001070112 spans an interval of 30 days) plus an extra 5 days for the last trajectories to be calculated to completion. There are 5 co-existing *sets* of trajectories at any one time ($n_s = T/\text{TRELEASE}$), giving much improved efficiency in the calculation (and in your time).

The distribution of particles at the time of release is controlled the namelist CLUSNAME (Table 5). Many of the controls here are not used for all of the release configurations, and when not used their values are ignored. You must choose what type of vertical coordinate you would like to release trajectories from (i.e. model level, pressure or isentropic surface) using INISURF. Many *clusters* of trajectories may be started at any one release time. Each cluster can be released on a different level (determined by ZCLUSTER).

The number of particles per cluster (n_c) depends upon the release configuration (e.g. for IPOSN=3, n_c = NXACR×NYACR). NPART should be set equal to the total number of co-existing trajectories = $n_s\times$ NCLUSTERS × n_c.

Consistency checks between the parameters NPART and IPTS and the namelist controls are made and sometimes erroneous namelist controls may be overridden. You should look in the output file (channel LOUTP) for all information on the interpretation of the namelist by the Offline package. This will help you construct a suitable jobdeck. Note that the largest array in the program contains all trajectory points (POSN) and has dimensions (IPTS, NPART, 3+NATTR). The number IPTS*NPART*(3+NATTR) influences the memory requirement of your job and the size of the output file. I would recommend keeping this number below 10^7.

The date of release is detailed in namelist DATENAME (Table 6) as is the filename prefix for the trajectory output. Note that since March 1999 the ECMWF analyses stored for UGAMP in /hold/badc by Paul Berrisford have four-digit years in the filenames and ISYY must contain four digits (e.g. 2001). Before this date two-digit years were used and these files will only be read correctly if ISYY contains those two digits (e.g. 96 rather than 1996).

If Unified Model data from several dumps (with interval THIST) are stored in a single daily file then you should ensure that NRECPFILE=1/THIST.

The remaining namelists, GRIBNAME, RSNAME and UMNAME (Tables 7, 8 and 9), are specific to wind records from ECMWF analyses, output from the Reading spectral model and output from the UKMO Unified Model respectively.

Trajectories can be output in two formats denoted by “ec” and “bin”. The “ec” format has the same form as used for the ECMWF special project back trajectories which are archived at BADC (see their World Wide Web page for details). This format is easy to interpret by eye. A sample header is given below:–

```
 TRAJECTORY BASE TIME IS 2000073112
 DATA BASE TIME IS 2000073112
 DATA INTERVAL IS    6 HOURS AND CONTAINS    6 TIMESTEPS
 TOTAL NUMBER OF TRAJECTORIES IS  2706
 NUMBER OF ATTRIBUTES IS    3
 ATTRIBUTE TYPES =
   1   3   4
 NUMBER OF CLUSTERS IS    2
 CLUSTER POINTERS =
       1    1354
 3D TRAJECTORY ? (T OR F): T
 FORECAST DATA ? (T OR F): F
 FORWARD TRAJECTORY ? (T OR F): F

 TRAJECTORY NUMBER    1 COMPRISES    2 INTERVALS

 STEP   HOURS  LAT         LON         P (MB)      ATTRIBUTES
    0    0.00  0.60000E+02  0.34800E+03  0.90000E+03  0.28034E+03  0.49746E+00  0.56815E-02
    6   -6.00  0.59608E+02  0.34995E+03  0.88926E+03  0.27937E+03  0.71189E+00  0.61785E-02
   12  -12.00  0.58989E+02  0.35062E+03  0.88716E+03  0.28028E+03  0.78777E+00  0.66582E-02

 TRAJECTORY NUMBER    2 COMPRISES    2 INTERVALS

etc.
```

The “bin” format is more compact but is largely obselete (see subroutine WRBIN for formatting details).

Name	Default	Purpose	Notes
NN	106	Total wavenumber truncation	Spectral records only.
MM	106	Zonal wavenumber truncation	Set to 1 for gridded input.
NHEM	2	Number of hemispheres	
NL	31	Number of levels in wind data	
MOCT	1	Imposed zonal symmetry	Spectral records only.
MG	320	Number of longitudes	For spectral records use
JG	80	Number of latitudes in a hemisphere	appropriate Gaussian grid.
NWJ2	2	Number of spectral coefficients	IUVFORMAT=1 only.
NCRAY	64	CRAY specific for FFT's	IUVFORMAT=1 only.
NTRAC	1	Number of tracers	Does not apply to ECMWF data but must always be ≥ 1.
NPART	1	Number of particle trajectories	Check against Tables 4 and 5.
IPTS	2	Number of points along a trajectory	See Table 4 for trajectory length.
NATTR	0	Number of attributes assigned	See Table 3.
MAXCLUS	10	Max number of clusters of particles	See Table 5.

Table 1: Fundamental parameters (in COMMON/PARAM1).

Channel name	Unit	Purpose
LOUTP	6	Information output by offline package.
INPUT	20	Input wind record.
INPUT2	21	Extra input (see Table 7).
NCBIN	2	Output trajectories in “bin” format.
NCEC	14	Output trajectories in “ec” format.
NCINTRAJ	12	Input particle release positions (IPOSN=7).
NCGP	40 $\rightarrow$ 39+MAXATTR	Scratch files containing attribute fields.

Table 2: FORTRAN IO Channels

Variable	Default	Purpose
IUVFORMAT	0	Format for wind records (including other fields):– 0: ECMWF records in GRIB format, 1: Reading spectral model history files, 2: UKMO Unified Model PP-files, 3: Other grid point records.
LSPECTRAL	.TRUE.	Is the input data spectral?
ILEVTYPE	0	Denotes vertical coordinate for input data. 0: $\eta \Rightarrow \dot{\eta}_{L+\frac{1}{2}}$ calculated for spectral records (IUVFORMAT=0,1). $\dot{\eta}_{L+\frac{1}{2}}$ input for gridded records (IUVFORMAT=2). 1: $p \Rightarrow \omega_L$ input. 2: Other coord, although p_L and ω_L must be input.
IWORDSIZE	8	Number of bytes per word (4 for workstations, 8 for CRAY).
LTRACSWITCH	.FALSE.	Tracer fields in record? Assumed false if IUVFORMAT=0.
KOLOUR (length NTRAC)	2	ONLY OPERATIVE IF LTRACSWITCH=.TRUE. Colours for tracer fields labelled 1 $\rightarrow$ NTRAC. Tracer initialised as:– 1: Potential temperature, 2: Potential vorticity, 3: Specific humidity.
IATTRTYP (length NATTR)	–	Array containing a code for each attribute assigned:– 0: Surface pressure (or surface geopotential for "llpr" data), 1: Temperature, 2: Potential temperature, 3: Ertel potential vorticity, 4: Specific humidity or relative humidity (data must be supplied), 5: Tracer field no. NCHI(1) from history record, 6: Tracer field no. NCHI(2) from history record.
NCHI (length 2)	1, 2	ONLY OPERATIVE IF LTRACSWITCH=.TRUE. Labels of tracers to be assigned as attributes.
LPOUT	.FALSE.	ONLY OPERATIVE IF ILEVTYPE=0 .TRUE. $\Rightarrow$ pressure output as vertical coordinate. .FALSE. $\Rightarrow$ η output as vertical coordinate.

Table 3: Namelist INPNAME; specification of contents of input data and attribute selection.

Variable	Default	Purpose
BEGDAY	0.	Day number of particle release (IUVFORMAT=1).
THIST	0.25	Interval (in days) between **wind** records.
LFORW	.TRUE.	.TRUE. ⇒ forward trajectory. .FALSE. ⇒ back trajectory.
NSTEPS	10	Number of integrator steps in interval THIST.
LEVERY	.FALSE.	.TRUE. ⇒ trajectory recorded every integrator step. trajectory length = (IPTS-1)*THIST/NSTEPS. .FALSE. ⇒ trajectory recorded at interval THIST. trajectory length = (IPTS-1)*THIST.
NSKIP	1	Output trajectory after every NSKIP trajectory records.
LMULTI	.FALSE.	.TRUE. ⇒ start "multiple" sets with staggered release times. .FALSE. ⇒ a single set of trajectories.
TRELEASE	0.25	ONLY OPERATIVE IF LMULTI=.TRUE. Interval (in days) between release of sets. NOTES (A) There maybe many "clusters" per "set". (B) Number of sets = trajectory length / TRELEASE. (C) NPART= # sets × # trajectories per set. (D) Each set is output as separate "ec" file labelled by its release date.
TINTEG	1.	ONLY OPERATIVE IF LMULTI=.TRUE. Total length of integration (in days).

Table 4: Namelist INPNAME; controls frequency of wind input, trajectory release times, time-stepping and trajectory output.

Variable	Default	Purpose
NCLUSTERS	1	Number of clusters of particles per set (see LMULTI). Must be $\leq$ MAXCLUS.
IPOSN	0	Release arrangement for each cluster:– 1: Particles on every grid point in horizontal on level ZCLUSTER, 2: Particles on every other grid point in horizontal, 3: Regular lon-lat rectangle (on level ZCLUSTER), 4: Regular lon-sin(lat) rectangle (on level ZCLUSTER), 5: Ball clusters, each containing a central particle surrounded by 6 others in 3D arrangement (INISURF=0 ONLY), 6: Isotropic, homogeneous pattern on a polar stereographic projection with MOCT-fold zonal symmetry (MOCT $\geq$ 2), 7: Particle positions are read in from channel NCINTRAJ. If you want to release trajs along a flight track you should also use the update interrel3.upd .
XCLUSTER	–	Longitude for NW corner of each cluster (IPOSN=3,4,5).
YCLUSTER	–	Latitude (or sin(lat)) for NW corner of each cluster (IPOSN=3,4,5).
ZCLUSTER	–	Level for each cluster: η for INISURF=0 and ILEVTYPE=0 p (10^5 Pa) for INISURF=0 and ILEVTYPE=1,2 p (10^5 Pa) for INISURF=1 θ (K) for INISURF=2 (not allowed if ILEVTYPE=2)
XSPACE	–	Spacing in longitude in degrees (IPOSN=3,4,5).
YSPACE	–	Spacing in latitude or sin(lat) (IPOSN=3,4,5).
ZSPACE	–	Spacing in vertical coordinate (IPOSN=5).
NXACR	–	Number of particles West-East (IPOSN=3,4).
NYACR	–	Number of particles North-South (IPOSN=3,4).
PHILIM	0.	Southernmost latitude for particles (IPOSN=6).
INISURF	0	0: Place particles on η surfaces (see ZCLUSTER), 1: Place particles on pressure surfaces, 2: Place particles on isentropic (θ) surfaces.

Table 5: Namelist CLUSNAME; release positions for clusters. Note that IPOSN $\rightarrow$ NYACR are arrays of length MAXCLUS.

Variable	Default	Purpose
ISYY	96	Year of release date.
ISMM	01	Month of release date.
ISDD	01	Day of release date.
ISHH	00	Hour of release date.
NRECPFILE	1	Number of wind records per input file.
FSTEMO	ec2d	Path and stem for files containing "ec" format trajectories.
IOFFOUT	5	Position in name string to write date. Determined in jobdeck.

Table 6: Namelist DATENAME; specifies release date and output filenames.

Variable	Default	Purpose
FSTEM	siua	Path and stem for filenames: upper air spectral records (LSPECTRAL=.TRUE.), gridded records on pressure levels (LSPECTRAL=.FALSE.).
FSTEM2	giua	Path and stem for filenames: specific humidity on Gaussian grid (LSPECTRAL=.TRUE.) (only used if after 4/4/95, or for ERA data), orography file (LSPECTRAL=.FALSE.).
IOFFSET	5	Position in name string to write date. Determined in jobdeck.
IDATADATE	96010100	Data base time (date that wind data is forecast). For "actual" analyses set IDATADATE = release date.
LERA	.FALSE.	ERA data? Used for reading specific humidity.

Table 7: Namelist GRIBNAME; for reading ECMWF records.

Variable	Default	Purpose
RNTAPE	1.	Run identification number.
TSPD	48.	Number of timesteps per day for history.
LDRY	.TRUE.	.TRUE. ⇒ No Q in history. .FALSE. ⇒ Q in history.
LT3D	.TRUE.	.TRUE. ⇒ History from RSGCM. .FALSE. ⇒ History from RSGUP3, BGCM5.

Table 8: Namelist RSNAME; for reading Reading spectral model history files.

Variable	Default	Purpose
YCPTHM	–	Directory containing input wind records.
YEXPUM	–	Experiment identifier.
YJOBUM	–	Job identifier.
YSUBUM	–	Submodel identifier.
YTIMUM	' . '	Timing in UM data.
YTYPUM	'p'	File type (e.g. PP-file).
YSTMUM	'a'	File-stream.
YEXT	'.pp'	Data filename extension.
LUARS	.FALSE.	UARS assimilation data?
LUARRM	.FALSE.	UARS running means?
LUM	.TRUE.	UM data?
LUMRM	.FALSE.	UM data (running means)?

Table 9: Namelist UMNAME; for reading Unified Model data.