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A Lagrangian Particle Dispersion Model Compatible with WRF

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1. Introduction

Lagrangian particle dispersion models (LPDMs) have been used for many years as a tool to simulate the transport and diffusion of atmospheric contaminants and determine source-receptor relationships. Mesoscale models are frequently used to provide the meteorological conditions that drive the LPDM. Since the Weather and Research and Forecasting (WRF) model is relatively new, there are no LPDMs that are currently compatible with WRF as far as we know. We have therefore adapted an existing LPDM called FLEXPART [*Stohl et al*., 2005] for use with WRF. An earlier version of FLEXPART has also been coupled with MM5 [e.g. *de Foy et al.,* 2006]. FLEXPART was selected because the code is well documented and it has many capabilities including the calculation of forward dispersion, backward response functions, trajectory clusters, removal processes, concentrations, uncertainties, age spectra, and mass fluxes.

FLEXPART is designed to perform particle dispersion computations based on wind fields derived from the ECMWF global forecast model; therefore, we have therefore made extensive modifications to the code so that

1) the particle position computations correctly utilize the native WRF grid,
2) the NetCDF output files produced by WRF are read directly, and
3) the assumptions employed by the model are consistent with mesoscale models rather than global models.

This paper summarizes the changes made to FLEXPART, that we now call FLEXPART-WRF, and presents an example simulation. The FLEXPART-WRF code should be considered a beta version. Although we have performed a number of tests, there may still be problems associated with certain configurations of the model that have not yet been checked. We also describe additional work needed to make FLEXPART-WRF more flexible and easier to use. The code is freely available via the main FLEXPART web site: http://zardoz.nilu.no/~andreas/flextra+flexpart.html.

2. Modifications to FLEXPART

FLEXPART is designed to use output from the ECMWF global forecast model defined on a latitude-longitude grid. Particle positions are computed using the same coordinate system. The coordinate system in WRF, however, is not defined in latitude and longitude but as either a Lambert conformal grid or polar stereographic grid. The u- and v-components of the wind in WRF are therefore not true east-west and north-south components. In FLEXPART-WRF, particle positions are computed using the map projection grid coordinate system, defined in meters, with the origin at the southwest corner of the outer nested domain. The release locations, particle positions, and concentration grid can also be specified using this coordinate system. However, the user is likely to still want to define release locations, particle positions, receptor locations, and concentration grid in terms of latitude and longitude. Both options are included in the code. When the latitude-longitude option is chosen, all horizontal positions are input and output as latitude and longitude (in degrees), but are converted to/from the grid meters coordinates system (which is always used for internal computation) using map projection routines.

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The reading of global forecast model output in grib format was replaced with NetCDF libraries so that WRF output files could be read directly. FLEXPART-WRF can utilize the meteorological quantities from multiple nested domains in two ways. First, all the nested domain results can be used by default. Particle positions are updated using the winds from the domain with the smallest grid spacing the particle is located. Second, the user can also use one particular nested domain if the application does not require meteorological conditions from the other nested domains. In theory, one could develop software that would manipulate the WRF NetCDF output files to produce binary files compatible with FLEXPART; however, this would introduce an extra task that would create unnecessary I/O computational time and make running FLEXPART less efficient.

A number of other features in the model have been changed for mesoscale applications. For example, FLEXPART parameterizes mesoscale wind velocity fluctuations derived from the ECMWF global forecasts and analyses. These wind components are now set to zero by default because the parameterization is not appropriate when using mesoscale simulation results. However, they can be turned back on for large-scale applications of WRF.

By default, FLEXPART computes u_*, PBL height, and (optionally) surface heat flux from the mean wind and temperature profiles. The user can still choose this method, but mesoscale models such as WRF usually compute these variables and it is more consistent to use the values predicted by WRF. The code will read the variables directly from the WRF output files. For this case, the user must check the WRF registry so that u_*, PBL height, and surface heat flux are written to the NetCDF output files. If FLEXPART-WRF cannot find these variables, the code will then assume they are missing and compute them by the default methodology.

Meteorological parameters from the ECMWF model's hybrid-pressure ("eta") levels are interpolated by FLEXPART to levels defined by a terrain-following Cartesian vertical coordinate. This simplifies the particle dispersion calculations, because the Cartesian level spacing does not vary horizontally. We chose to retain this feature in FLEXPART-WRF, although several modifications were made to account for the differences between ECMWF and WRF. For example, vertical velocities in ECMWF output files are terrain following and in "etadot" units whereas WRF vertical velocities are full vertical velocities in m s^{-1}.

To enable trajectories to be calculated with the FLEXPART-WRF code, we have also added a parameter that turns off the turbulent wind components in the computing of particle positions.

3. Example Results

To test the trajectory, particle dispersion, and concentration field computations, we employed WRF simulations of circulations over central Mexico. This region was chosen because the large elevation variations will challenge the assumptions and interpolation associated with the vertical coordinate. WRF was run with three nested domains: the outer grid encompassed Mexico with a grid spacing of 22.5 km while inner nested grids were centered over Mexico City with grid spacings of 7.5 and 2.5 km.

A series of FLEXPART-WRF runs were performed to simulate the multi-day dispersion of pollutants emitted from Mexico City between 26 February and 4 March 1997. The first run continuously released 10,000 particles from a 1225 km^2 box in the Mexico City valley between 06 and 18 LST 26 February. For the second run, particles were released during the following 12-h period between 18 LST 26 February and 06 LST 27 February. The rest of the runs released particles during subsequent 12-h intervals until 06 LST 2 March. In this way, the multi-day particle plume can be segregated by release time that corresponds to daytime and nighttime release periods.

Figure 1 shows the predicted particle positions during the evening at 06 UTC 28 February 1997 from both a regional and local perspective. The synoptic winds were primarily southwesterly during the period so that the particle plume was transported to the northeast. During the daytime, particles were mixed within the convective boundary layer up to 2-3 km AGL over Mexico City. As the ambient mid-troposphere winds transport the particles to the northeast, the plume became decoupled from the surface over the Gulf of Mexico. The decoupling produced layers in the mid-troposphere that were often relatively thin. While particles were transported relatively quickly out of the central plateau, a wide distribution of particles from daytime and nighttime periods mixed together over the Gulf of Mexico. Note that the center of mass computations (dots) are based on only those particles within the computational domain; therefore, some caution should is warranted when a large fraction of the particles have been transported out of the domain.

Figure 2 is a plot of the concentrations resulting from the particle positions at 06 LST 28 February that correspond to Fig. 1a. A uniform kernel is used to compute concentrations that smooth out some of the spatial variations in the particle plume.

The user can also evaluate how different configurations of WRF affect transport and diffusion. For example, WRF simulations were completed that were identical except for the choice of PBL parameterization. An example of the results is shown in Fig. 3. While the particle plumes from both simulations are qualitatively similar, there were subtle differences in the wind and temperature fields that produced differences in the particle concentration and spatial distribution of particles. For this period, the particle plume from the YSU PBL simulation downwind of Mexico City was more diffuse that the plume produced by the MYJ PBL simulation.

4. Future Direction

We have tested the FLEXPART-WRF using the primary capabilities of the code including:

- Forward / backward dispersion
- Forward / backward trajectories
- Receptor concentrations
- Clustered trajectories

Forward simulations have been more thoroughly tested than backward simulations. Additional testing is needed to thoroughly test other capabilities of the code including emission variation files, removal processes, uncertainties, age spectra, mass fluxes, and the simulation of atmospheric trace gases such as stratospheric ozone.

The beta version of FLEXPART-WRF should work for most forward/backward trajectory and dispersion applications. Nevertheless, our experience with the code has identified several issues that should be addressed for long-term use of FLEXPART-WRF including:

1) Graphical Output: There is currently no graphical user interface (GUI) for FLEXPART. All of the output is produced by binary or ascii files and the user must provide the software to plot the results.
2) Turbulence: Turbulent wind components are currently calculated using the parameterizations described in *Stohl et al.* [2005]. It would be useful to have the option of making the turbulent components consistent with turbulence kinetic energy predicted by WRF.

3) Testing of Input Options: Additional tests are needed to identify combinations of input options with the WRF-specific modifications to the code.
4) Near-surface meteorological quantities: FLEXPART computes 10-m winds and 2-m temperature based on the coarse resolution output from the ECMWF model. An option needs to be added to deactivate this when the mesoscale model simulation has fine vertical grid spacings near the surface.
5) Computational Efficiency: Our experience is that the trajectory and particle dispersion in FLEXPART-WRF predictions take longer than one would expect. This is mostly likely related to I/O associated with the NetCDF files and other output format types in WRF should be evaluated.

We are currently working on these five issues and expect another version of FLEXPART-WRF to be available this fall.

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6. References

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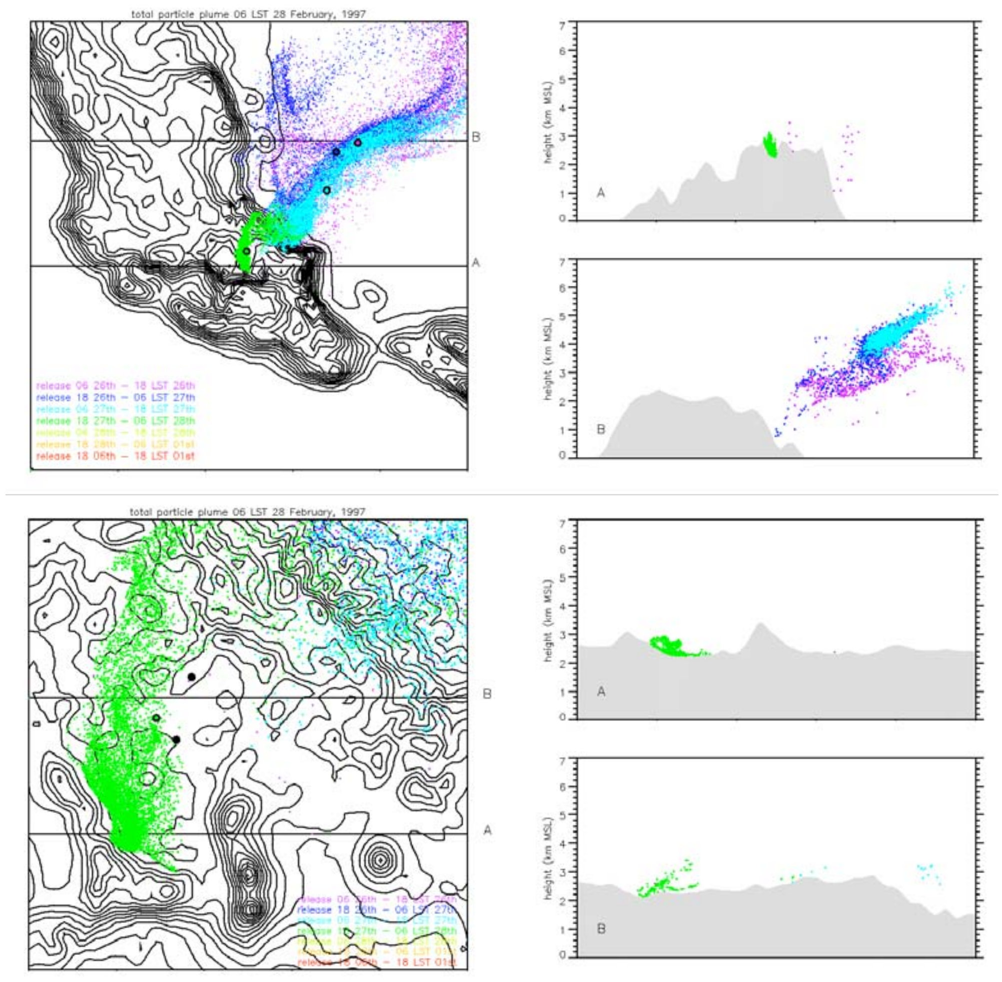

Fig. 1. Simulated particle plume at 06 LST 28 February from a regional (top) and a local (bottom) perspective. The spatial extent of the plots corresponds to domains 1 and 3 for the regional and local perspectives, respectively. Black contours denote topography and the color of small particles denote the release period. In the X-Y plots (left, the large

filled colored circles denote center of mass of the particle plume. Particles within 22.5 km and 2.5 km of lines A and B are shown in the vertical cross sections (right).

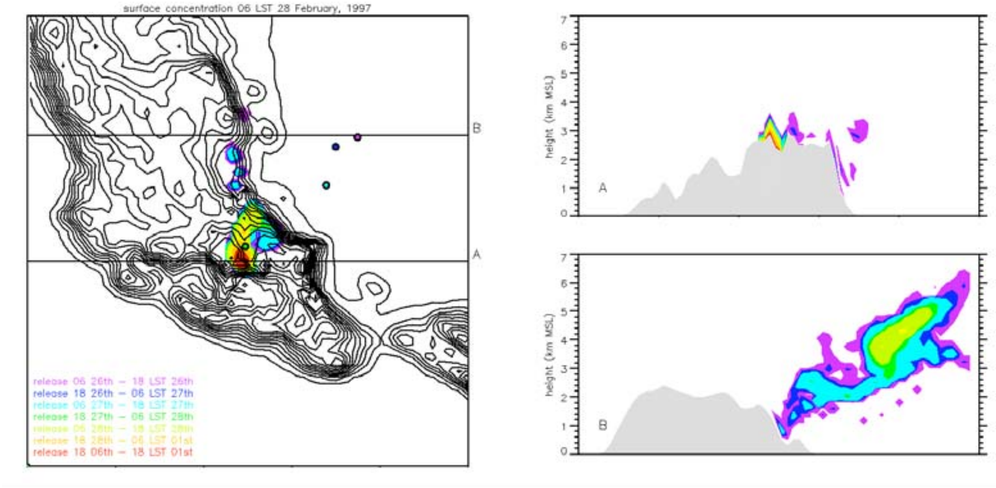

Fig. 2. Same as Fig. 1 (top), except concentrations derived from the particle plume is shown.

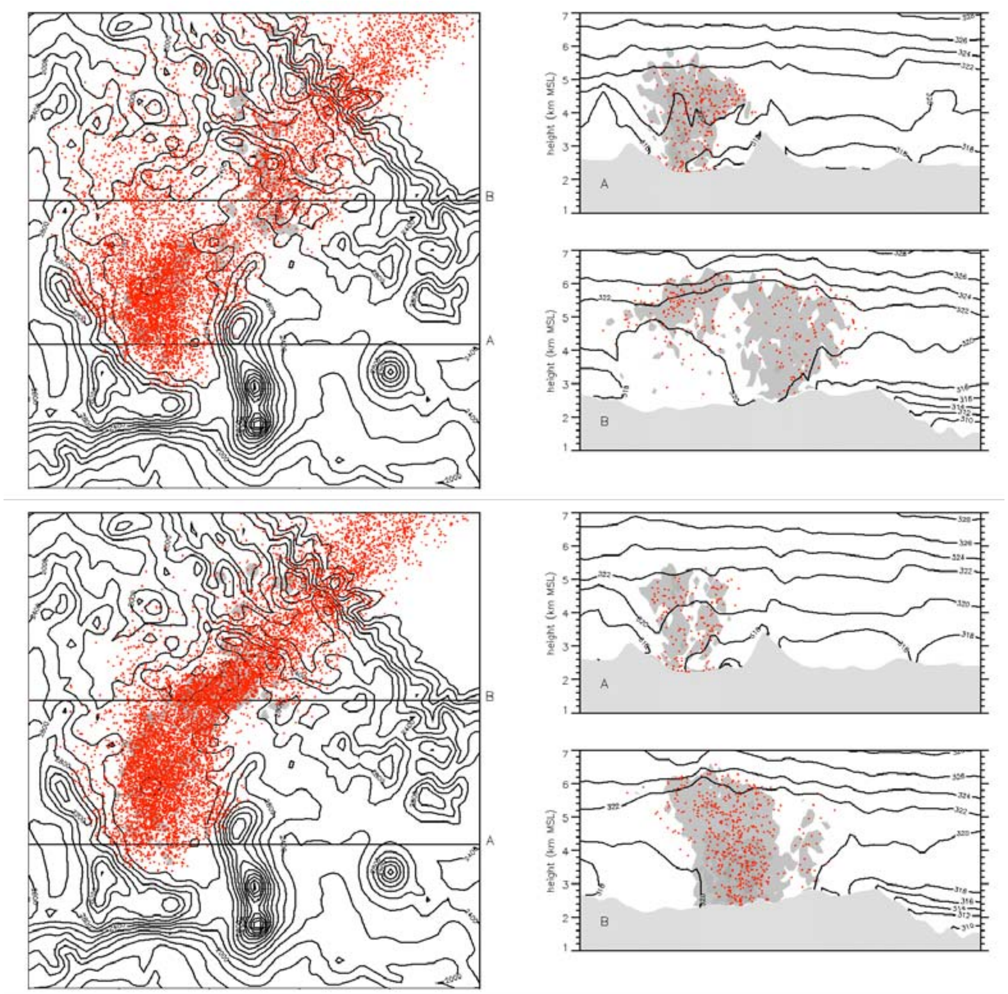

Fig. 3. Comparison of forward dispersion over central Mexico at 18 LST 1 March 1997 using the YSU (top) and MYJ (bottom) PBL parameterizations in WRF. Gray shading denote particle concentration at the surface (left) and along the vertical cross sections (right). Black contours denote topography (left) and potential temperature (right).