universität wien

Revamping FLEXPART for the next generation of simulations

Lucie Bakels, Marina Dütsch, Katharina Baier, Silvia Bucci, Andreas Plach, Daria Tatsii, Andreas Stohl, and Martin Vojta

FLEXPART general overview

- Lagrangian trajectory model
- Running on meteorological input data
- Used for i.e.:
  - Aerosols
  - Inverse modelling of greenhouse gases
  - Global moisture and heat transport
- Two main improvements:
  - Accuracy (ECMWF input data)
  - Speed (in case of long global runs with many particles)

Native ETA coordinate system (ECMWF)

- FLEXPART converts native ECMWF vertical ETA levels to vertical levels in meters
- Reason: turbulence in boundary layer

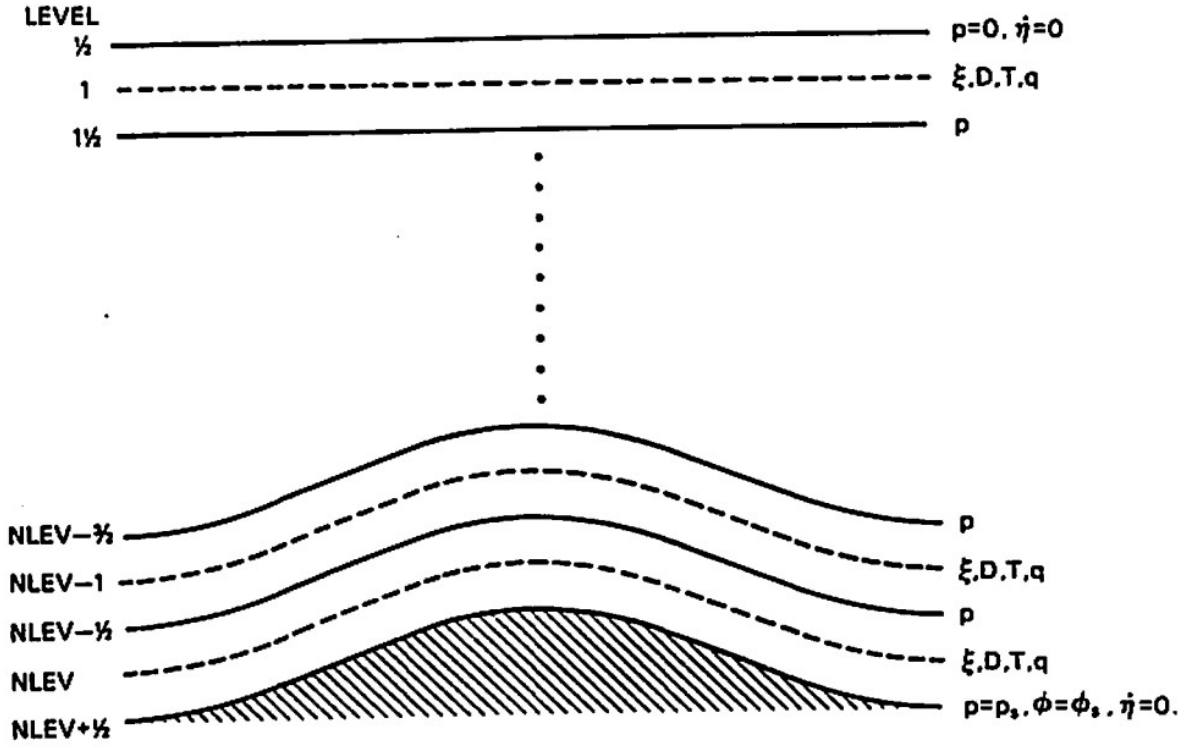


Fig. 2.3 Vertical distribution of variables

ECMWF research manual 1988

Native ETA coordinate system (ECMWF)

- Interpolation between the ETA and meter levels causes extra errors
- Gridded properties do no longer need to be internally converted to meter units above the boundary layer
- Optional (can be switched off)

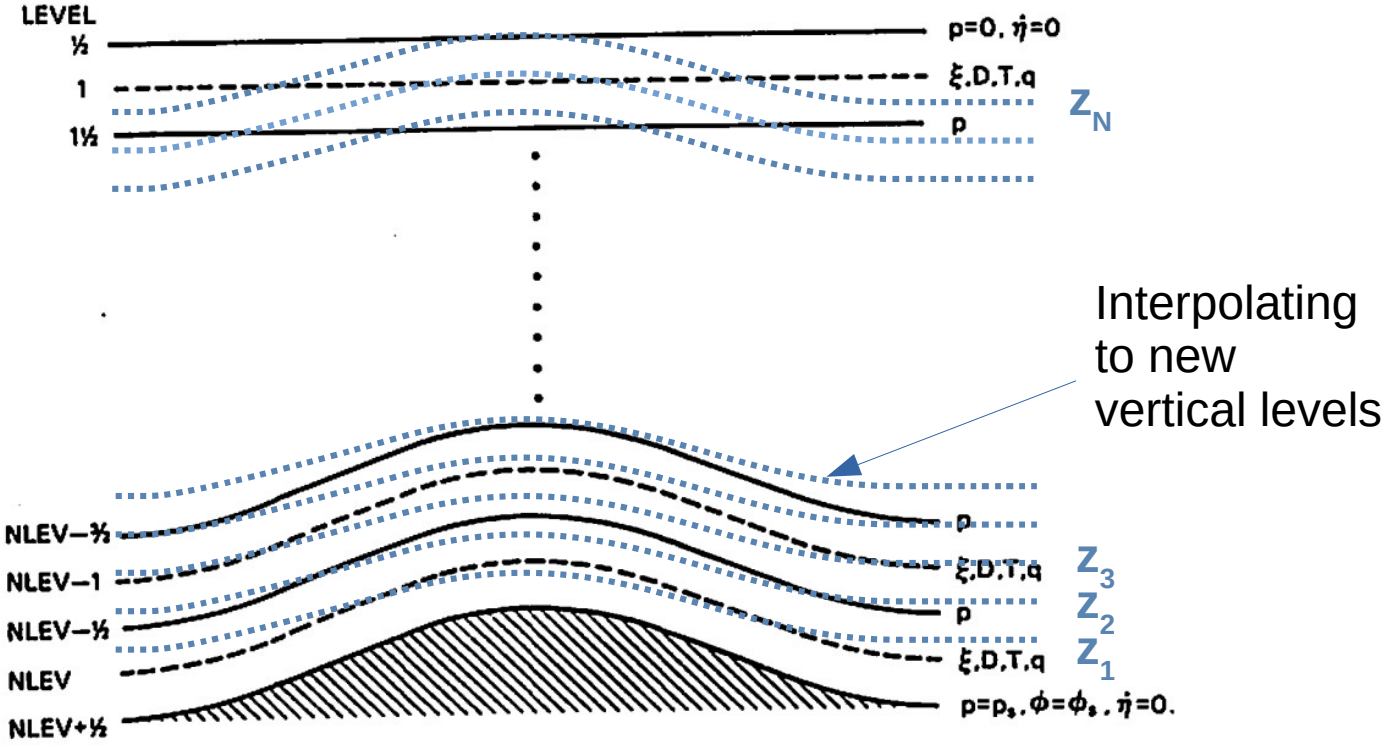


Fig. 2.3 Vertical distribution of variables

ECMWF research manual 1988

Improvements: conservation of semi-conserved properties along trajectories

Absolute and relative tracer conservation errors of:

- Potential vorticity
- Potential temperature
- Specific humidity

$$ATCE(t) = \frac{1}{N}\sum_{n=1}^{N} |T_n(t) - T_n(0)|$$

Tracer along trajectory n

$$RTCE(t) = \frac{\sum_{n=1}^{N} |T_n(t) - T_n(0)|}{\sum_{n=1}^{N} \frac{1}{2}|T_n(t) + T_n(0)|}$$

Improvements: conservation of semi-conserved properties along trajectories

Absolute and relative tracer conservation errors of:

- Potential vorticity
- Potential temperature
- Specific humidity

$$ATCE(t) = \frac{1}{N}\sum_{n=1}^{N} |T_n(t) - T_n(0)|$$

Tracer along trajectory n

$$RTCE(t) = \frac{\sum_{n=1}^{N} |T_n(t) - T_n(0)|}{\sum_{n=1}^{N} \frac{1}{2}|T_n(t) + T_n(0)|}$$

Maximise conservation by particle selection (avoiding clouds and PBL):

- Latitude: between ±40°and ±80°
- Relative humidity: below 90%
- Above the PBL

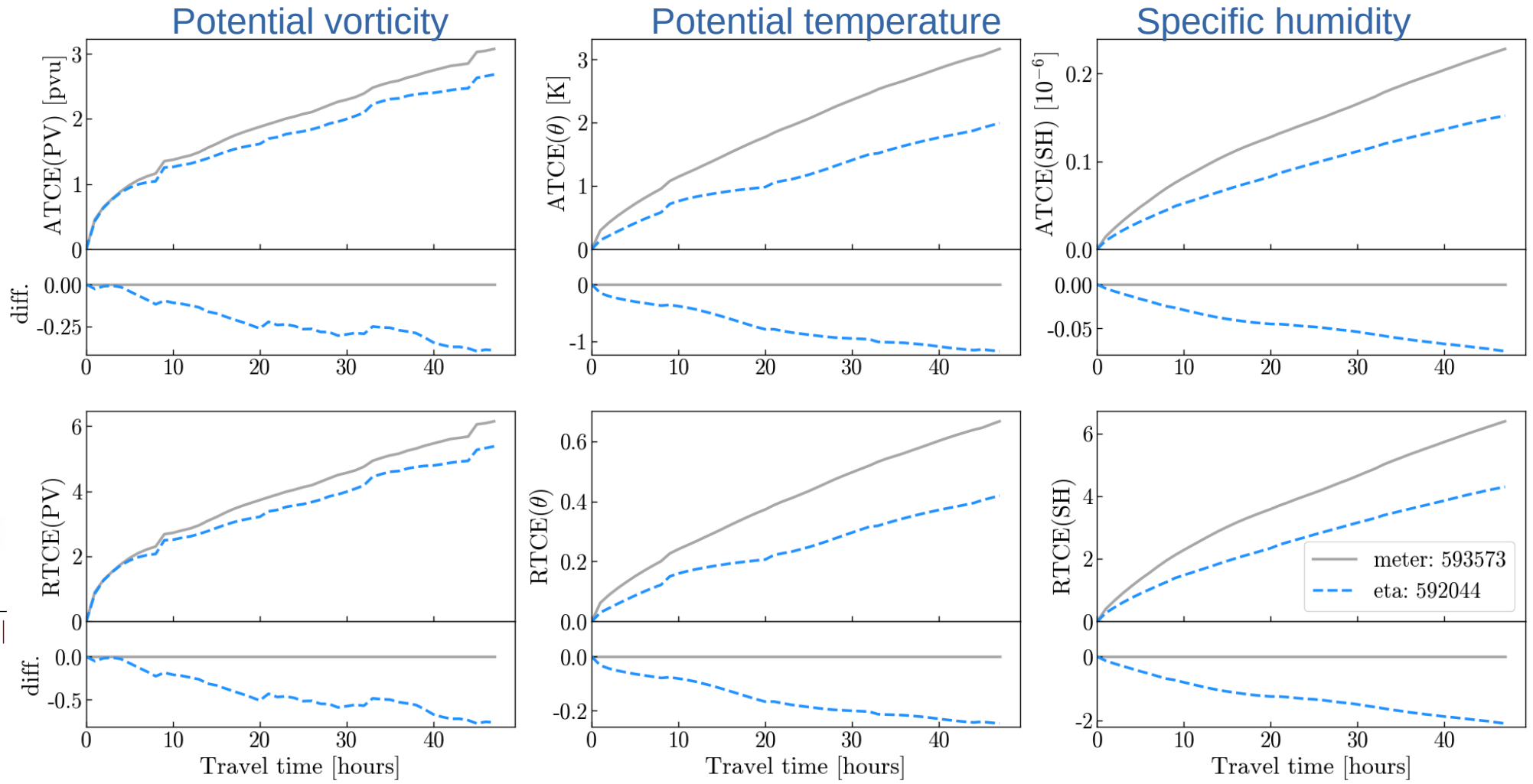
Improvements: conservation of semi-conserved properties along trajectories

Maximise conservation by particle selection:

- Latitude: between ±40°and ±80°
- Relative humidity: below 90%
- Stratosphere: 10 to 50km

$$ATCE(t) = \frac{1}{N}\sum_{n=1}^{N} |T_n(t) - T_n(0)|$$

$$RTCE(t) = \frac{\sum_{n=1}^{N} |T_n(t) - T_n(0)|}{\sum_{n=1}^{N} \frac{1}{2}|T_n(t) + T_n(0)|}$$



Improving speed: OpenMP parallelisation

Following FLEXPART CTM, parallelisation covers:

- Reading windfields
- Convection calculations
- All particle based computations

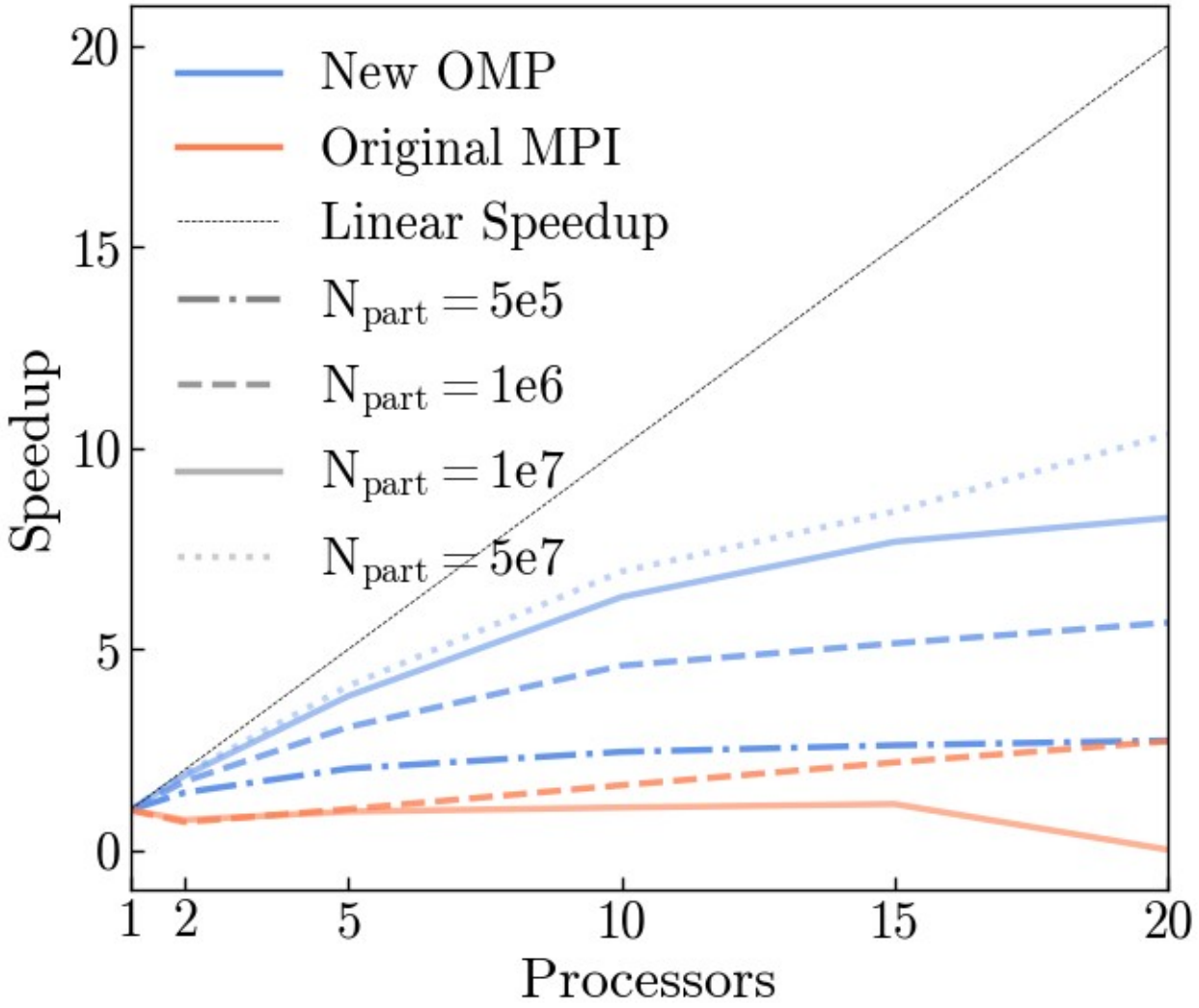
Improving speed: OpenMP parallelisation

Following FLEXPART CTM, parallelisation covers:

- Reading windfields
- Convection calculations
- All particle based computations

Airtracers distributed around the whole globe using ERA5:

- Improvement when comparing to the original MPI
- Speedup varies greatly for different simulation set-ups
- **Work in progress!**



universität wien

- Increased accuracy
- OpenMP parallelisation

Other improvements

- Increased readability
  - Organised the code using modules
  - Introduced functions and subroutines to reduce double code
- Particle dump in NetCDF format
  - ~30% smaller files than binary
  - Fields can be chosen by input option file

Stay tuned for the official release!

lucie.bakels@univie.ac.at