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Eidgenössisches Departement des Innern EDI
Bundesamt für Meteorologie und Klimatologie MeteoSchweiz

FLEXPART for COSMO and ICON

COSMO GM 2023 WG4

Pirmin Kaufmann, Stephan Henne

Differences IFS/GFS to COSMO

- Horizontal coordinates: regular versus rotated latitude-longitude grid
- Vertical coordinate system: hybrid-pressure versus several options in COSMO
- Vertical wind representation: eta-dot versus w relative to horizontal plane
- Differing GRIB code tables
- Non-staggered versus staggered grids for wind

→ The many fundamental differences require a separate source code for FLEXPART-COSMO

FLEXPART-COSMO

Henne, S., Brunner, D., Oney, B., Leuenberger, M., Eugster, W., Bamberger, I., Meinhardt, F., Steinbacher, M., and Emmenegger, L. , 2016: Validation of the Swiss methane emission inventory by atmospheric observations and inverse modelling, Atmos. Chem. Phys., 16, 3683–3710, https://doi.org/10.5194/acp-16-3683-2016.

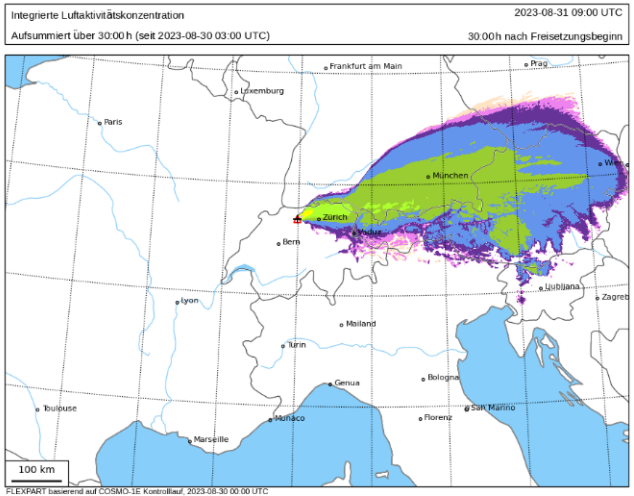
- Derived by Empa (Dominik Brunner, Stephan Henne) from FLEXPART v 8.0
- OpenMP parallelization and reformatting in f90 free format by MeteoSwiss (Martin Schraner, Pirmin Kaufmann)
- Maintained and regularly updated by Empa

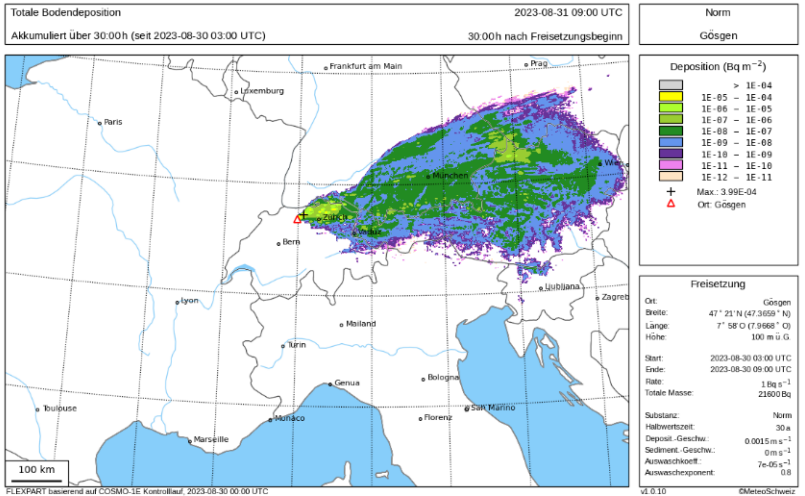
FLEXPART-COSMO

- Recent updates by Empa:
  - Modified turbulence scheme for high resolution COSMO (< 3 km)
  - Control input files (COMMAND, etc.) in Fortran namelist format
  - Additional INPUT_PHY namelist with settings for PBL determination, turbulence scheme, landuse file, originating institution

Operational Use at MeteoSwiss

Regular deterministic runs every 3 hours for 6 locations, based on COSMO-1E Control



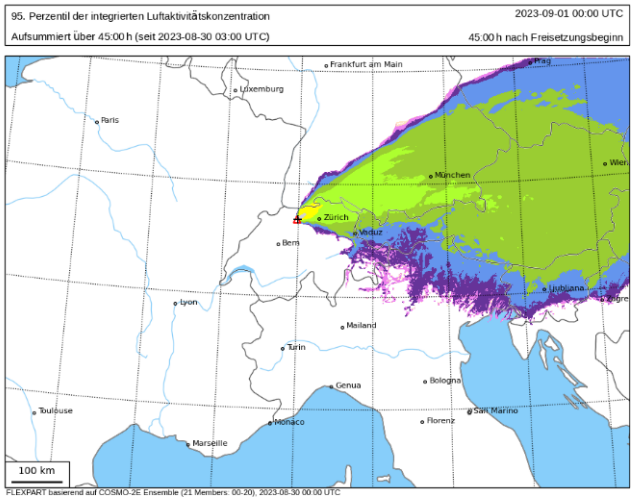


Integrated Conc. (30 h after release)

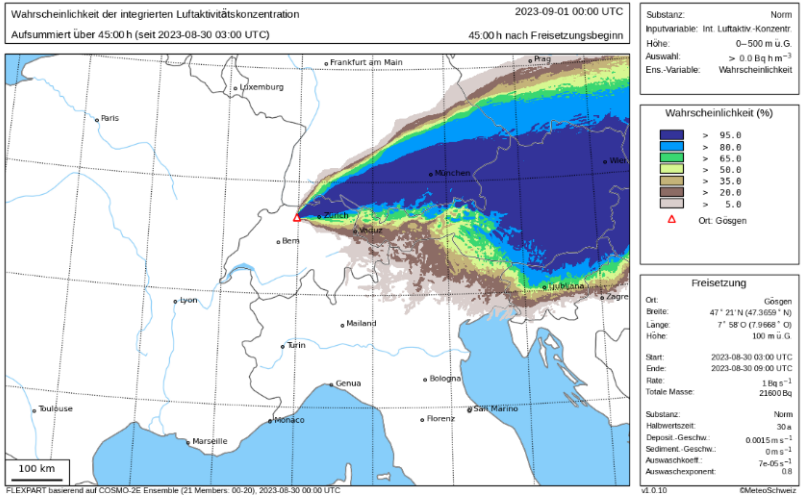
Deposition (30 h after release)

Operational Use at MeteoSwiss

Regular ensemble runs every 6 hours for 6 locations, based on COSMO-2E Ensemble with 21 members



95% Quantile of integ. conc. (45 h after release)



Probability (45 h after release)

FLEXPART-ICON

- FLEXPART for ICON is the next step of development by Empa (Stephan Henne)
- Use of ICON model output on native triangular grid
- Interpolation with adapted version of icontools library

Trajectory Prototype

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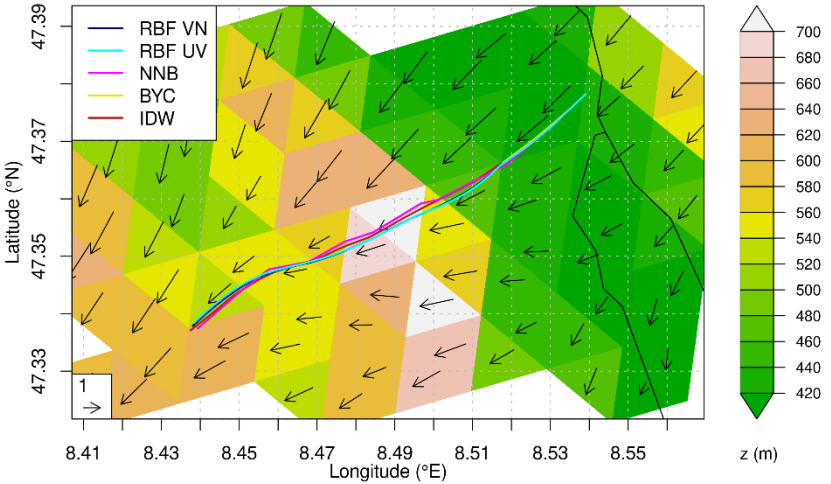
- Standalone: no more dependencies from other libraries (MPI codes)
- Derived types for icon grid, RBF routines largely taken from icontools (license issue?)
- Extended to facilitate interpolation to individual points
- Interpolation methods
  - Scalars: next neighbour (**NNB**), barycentric (**BYC**), radial basis functions (**RBF**), inverse distance weight (**IDW**)
  - Edge-normal wind: **RBF-VN** only
- Localisation method
  - Poor man's approach: check all cells
- Particle tracking
  - Keep geographic location and grid indices in memory
  - Search only cell and neighbours after location upate



Simple forward trajectory integration in stationary wind field (forward Euler)
Time step: 120 s
Simulation period: 2 h

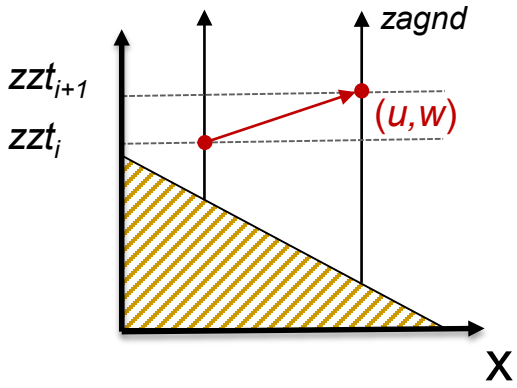
All methods ~~(except byc)~~ technically work
Very reasonable visual agreement with wind field
Only small differences between methods (simple case)

Contravariant Vertical Wind Correction

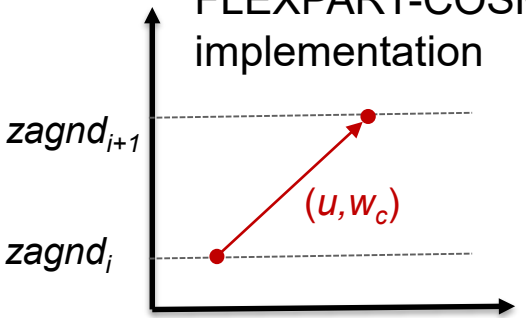
- Vertical wind output from ICON is given relative to height above sea level
- In FLEXPART-COSMO vertical wind relative to surface is required
- Contravariant wind correction of vertical wind is given by (Zängl et al., 2014)

$$w_{cc} = v_n \frac{\Delta h}{\Delta n} + v_t \frac{\Delta h}{\Delta t} .$$

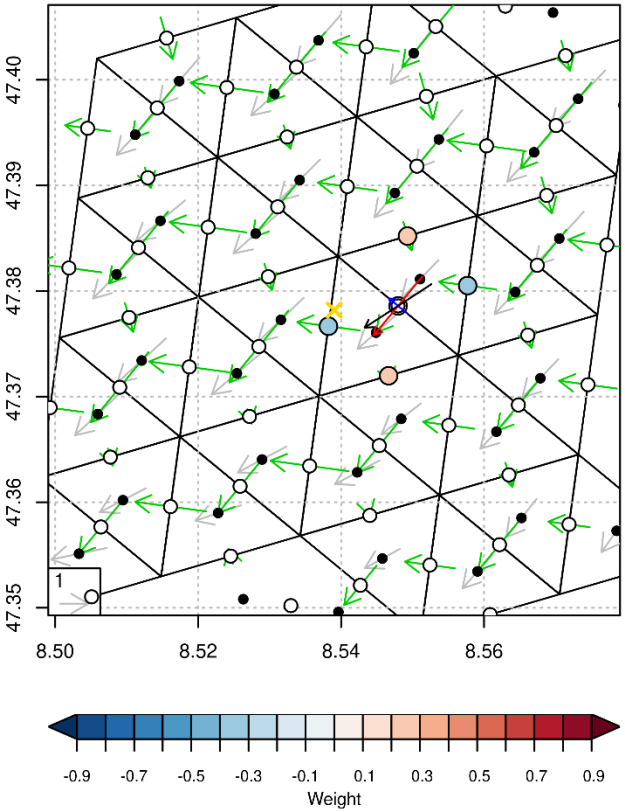
- v_n and v_t are the edge-normal and edge-tangential horizontal wind components
- $\Delta h/\Delta n$ and $\Delta h/\Delta t$ are the level height gradients (normal and tangential to edges



FLEXPART-COSMO implementation



Four Point RBF Stencil for VT Reconstruction



Gray: U,V @ cell centers
Green: VN @ edge centers

Blue: VT @ destination edge, reconstructed from VN at 4 point stencil (coloured points)
Red: VN @ destination edge, reconstructed from VN at 4 point stencil (coloured points)

In the plot: Scaling for U,V vectors slightly differs from others!

(See Zängl et al., 2014)

Wind Input & Interpolation Options

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- **U, V** (@ cell centers) required for interpolation to particle position
- **VN, VT** (@ edge centers) required for contravariant wind correction

- **VN, U, V** in ICON output
  - Calculate VT field every time new file is read
  - Interpolate from U, V to particle (scalar)
- **VN** in ICON output
  - Calculate VT, U, V field every time new file is read
  - Interpolate from U, V to particle (scalar)
- **VN** in ICON output
  - Calculate VT field every time new file is read
  - Interpolate from VN to particle (vector)
- **U, V** in ICON output
  - Calculate VN, VT every time new file is read
  - Interpolate to particle from U, V (scalar)
- For flexibility implement all 4?

FLEXPART-ICON versus FLEXPART-COSMO

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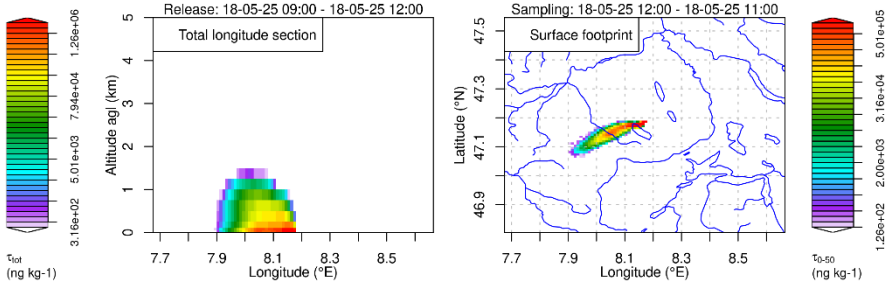
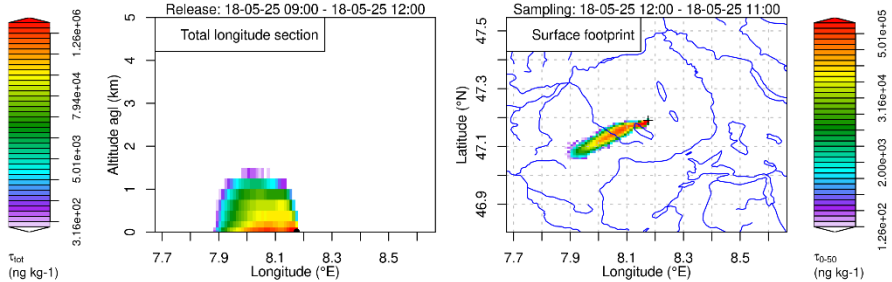
Starting from same ICON run

direct use of ICON output



Runtime: 220 s (debug, 8 threads)
90 s (opt, 8 threads)

ICON->COSMO using BYC



Runtime: 109 s (debug, 8 threads)
35.7 s (opt, 8 threads)

Next Steps

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- Selection of interpolation type (scalar, vector) for ICON (idw hardwired right now)
- Calculation of U, V from VN, to avoid storing/reading separate fields
- Calculation of VN, VT from U, V in case VN was not stored
- Tuning of stencil inquiries (avoid superfluous calculations)
- Tuning of stencil/weight calculations (precision?, icontools using double precision)
- RBF scale? How to set it in a useful way?
- Tree method for finding containing triangle (from icontools?)
- Domain issues: end particle for LAM, test global ICON inputs

- Convection requires modification! Sorting of particle locations, use of indices, loop over grid cells with particles, etc. …
- ohreaction still contains un-treated interpolation
- Not all "_nest" routines touched yet (required?)
- Output on icon grid (required?)

- Test simulations to determine best interpolation strategy (accuracy vs. costs)

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