Lagrangian transport modeling with FLEXPART

Practical Environmental Measurement Techniques

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Different kinds of atmospheric models

Atmospheric composition modeling

In order to properly simulate atmospheric composition / atmospheric chemistry, the following processes need to be represented:

- dynamical processes that drive atmospheric transport
- chemical processes of atmospheric constituents
- radiative processes that drive photochemistry and climate forcing
- emissions from anthropogenic and natural processes
- evolution of aerosol particles and their interactions with clouds
- exchange with surface reservoirs / biogeochemical cycling

Eulerian and Lagrangian atmospheric models

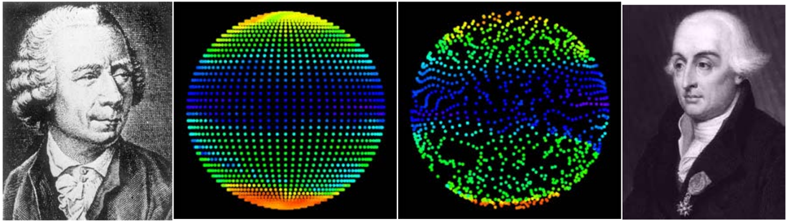

Figure 1: Global trace species concentrations, from a Eulerian (left) and Lagrangian (right) model (from: Brasseur and Jacob 2017)

Eulerian model:

- Leonhard Paul Euler
- fixed computational grid
- grid boxes have an air mass which has properties
- observer remains stationary at fixed grid points, observes state variable Ψ

Lagrangian model:

- Joseph Louis, Comte de Lagrange
- ensemble of air parcels which have properties
- air parcels move with airflow
- tracks state variable(s) Ψ of the air parcel as it moves in the atmosphere

Eulerian atmospheric models: Principle

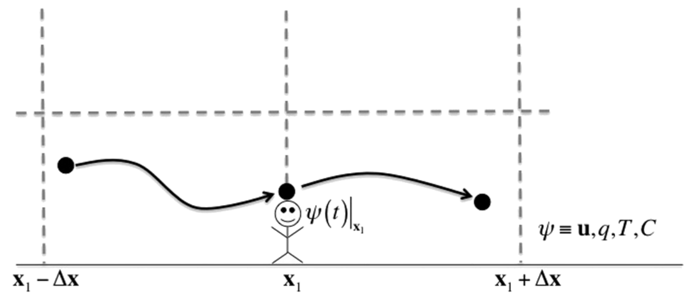

Figure 2: Eulerian modeling principle (from: Lin 2013)

- state variables ψ are calculated *at discrete grid points*
- locations *in between grid points* → interpolation
- but: result is *gapless* representation of the whole model domain
  → good for getting state of atmosphere *as a whole*
- trace gas concentrations are just further state variables (all species' concentrations available in all boxes) → *full chemistry simulations* possible

Eulerian atmospheric models: Mathematical formulation

- In the Eulerian reference frame, a state variable Ψ (e.g., temperature, pollutant concentration, humidity, wind, …) is described by

$$\frac{\partial \Psi}{\partial t} + \boldsymbol{u} \cdot \nabla \Psi = S$$

- S are all relevant source terms:
  - Ψ is *temperature* $\rightarrow$ S is *diabatic heating*, *radiative cooling*, …
  - Ψ is *velocity* $\rightarrow$ S is *pressure gradients*, *Coriolis force*, …
- $\frac{\partial(\ldots)}{\partial t}$ represents the rate of change *at a fixed position*, and ∇ is the *spatial gradient operator* at the same position.
- $\boldsymbol{u} \cdot \nabla \Psi$ is the non-linear *advection term*

Eulerian atmospheric models: Use cases

Some example uses of Eulerian atmospheric models:

- Numerical weather prediction model → *weather forecast*
- General circulation model → *climate modeling*
- Atmospheric chemistry model → *air quality modeling*

Lagrangian atmospheric models: Principle

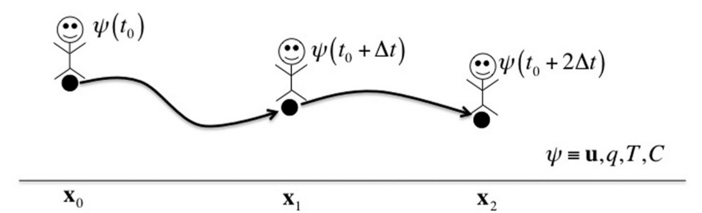

Figure 3: Lagrangian modeling principle (from: Lin 2013)

- ensemble of *air parcels*, observer “moves” with airflow, tracking state variable(s) ψ
- explicit link of an air mass with its past / future
- no interactions between air parcels
- limited loss processes possible (decay, deposition, OH reaction)
- usually not used for full chemistry simulations

Lagrangian atmospheric models: Mathematical formulation

In the Lagrangian viewpoint, the *state variable* Ψ for an air parcel changes as

$$\frac{D\Psi}{Dt} = S$$

- $\frac{D(\dots)}{Dt}$ is the *Lagrangian* or *total* derivative ($\frac{D\Psi}{Dt} = \frac{\partial\Psi}{\partial t} + \frac{\partial\Psi}{\partial x}\frac{dx}{dt} + \frac{\partial\Psi}{\partial y}\frac{dy}{dt} + \frac{\partial\Psi}{\partial z}\frac{dz}{dt}$)
    - coordinates are *parameters* of an air parcel (i.e., the observer), not fixed
    - represents rate of change *following the air parcel*
- S are *source terms*:
    - Ψ is *temperature* $\rightarrow$ S is *diabatic heating*, *radiative cooling*, …
    - Ψ is *velocity* $\rightarrow$ S is *pressure gradients*, *Coriolis force*, …

What can a Lagrangian model do?

- ~~dynamical processes that drive atmospheric transport~~ (has to be used as input)
- ~~chemical processes of atmospheric constituents~~ (only very limited, see below)
- ~~radiative processes that drive photochemistry and climate forcing~~
- emissions from anthropogenic and natural processes
- ~~evolution of~~ aerosol particles and their interactions with clouds (only one-way, i.e., wash-out by precipitation)
- ~~exchange with surface reservoirs / biogeochemical cycling~~
- atmospheric transport using the provided wind fields

> A Lagrangian model can only do a very limited set of things, but *when* it can be used, it's a great tool!

Lagrangian atmospheric models: Use cases

Some example uses of Lagrangian transport models:

- assess impact of emission events (e.g., wildfires, nuclear incidents, power plants, …)
- determine source regions of measured air masses
- determine contribution of individual emission sources to measured concentrations
- quantify emission fluxes of trace gases

… but all this only for chemically “simple” species, i.e., without complex interactions

The concept of “air parcel”

Dandelion seeds as ’air parcels’

Figure 4: source: Flickr.com (run movie 1 | run movie 2)

What is an air parcel? (more formal description)

- often used concept in atmospheric science
- a “chunk” of the atmosphere that is
    - large enough to encompass enough molecules to possess well-defined properties:
        - density
        - temperature
        - humidity
        - pollutant concentration
    - small enough such that the parcel can be thought of as occupying an *infinitesimal location* in space
- similar to the concept of *point mass* or *frictionless billiard ball* commonly encountered in introductory physics
- can carry a *mass* of a *trace gas* or *aerosol*

Air parcels in *Lagrangian particle dispersion models*

- air parcels are transported with *random velocities* to simulate turbulence
- often tracking many thousands (or even millions) of particles in three dimensions
    - capture stochastic effects of turbulence

Figure 5: (source: VectorStock.com/14263149)

How to run a Lagrangian model?

Meteorological input

- wind fields are *not* calculated by the Lagrangian model
- instead, use meteorological fields from Eulerian model:
    - operational numerical weather prediction model
    - general circulation (i.e., climate) model
    - mesoscale (i.e., regional) weather prediction model
- interpolate meteorological fields to location of air parcel
- needed parameters:
    - wind (horizontal and vertical)
    - mixing height (i.e., vertical extent and intensity of mixing within the PBL)
    - temperature
    - humidity
    - cloud properties
    - surface properties
- quality of meteorological fields of critical importance

Note

A Lagrangian particle dispersion model simulates atmospheric *transport* and needs wind fields *from external sources*.

Forward-time simulations

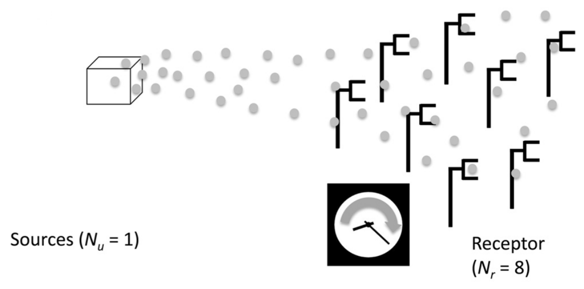

Figure 6: Forward-time Lagrangian particle dispersion model (from: Lin 2013)

- follow an air parcel *forward* in time, i.e.,

$$\boldsymbol{x}(t_0 + \Delta t) = \boldsymbol{x}(t_0) + \boldsymbol{u}(t_0) \cdot \Delta t + \dots$$

- efficient when looking at
    - only few sources / release points
    - multiple targets / receptors

Backward-time simulations

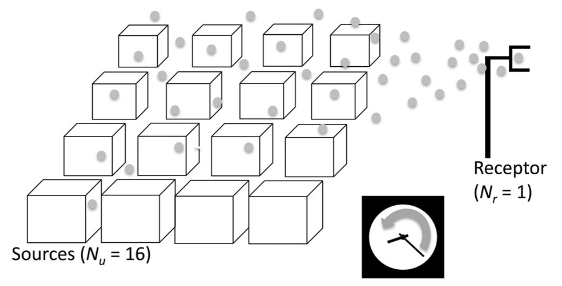

Figure 7: Backward-time Lagrangian particle dispersion model (from: Lin 2013)

- start at *receptor*, follow the air parcel *backward* in time, i.e.,

$$\boldsymbol{x}(t_0 - \Delta t) = \boldsymbol{x}(t_0) - \boldsymbol{u}(t_0) \cdot \Delta t + \dots$$

- determine sources of observed air masses → emissions
- is significantly more efficient when *#(receptors) « #(sources)*

Forward-time vs. backward-time simulations

Forward-time	Backward-time
Where does the air *go*?	Where does the air *come from*?
What is the *downwind* impact of air *coming from* a source?	What are the *upwind* influences on a region of interest?
Where do tracers get transported?	Where are the source regions of tracers?
How much is the tracer concentration at *downwind* locations affected by a unit emission from the source?	How strong is the *sensitivity* of the receptor to a particular *upwind source region*?

Output of a Lagrangian model

The *internal model state*

Figure 8: Individual particle positions (after: Lin 2013)

- the model's internal variables are *x*, *y*, *z*, and *mass* for every air parcel and time step
- physically most accurate, but difficult to interpret

Mean trajectory output

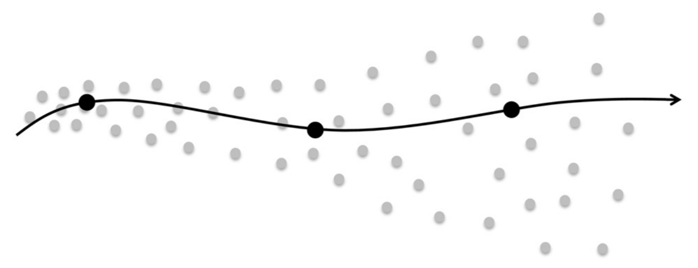

Figure 9: Calculation of mean trajectory (from: Lin 2013)

- output (weighted) average location of all air parcels: $x(t)$, $y(t)$, $z(t)$ at each time step
- easy to understand
- often not very accurate (imagine obstacles)

Gridded concentration output

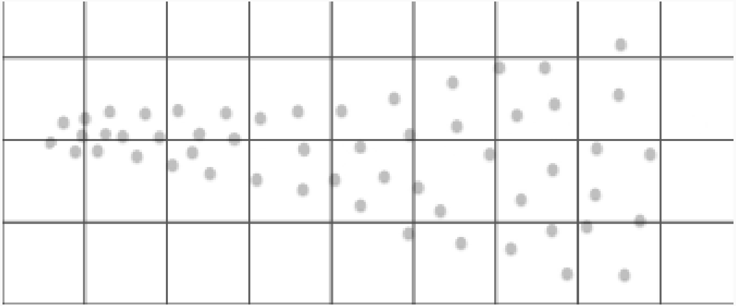

Figure 10: Gridded concentration output, simplified to 2-D (after: Lin 2013)

- define a grid (lat×lon×z)
- at each time step and for each grid cell, calculate mean mass density ($\frac{ng}{cm^3}$) from all air parcels within the cell
- air parcels remain unchanged, only the output is gridded!
- additionally: *gridded deposition output* (see below)

Gridded output from backward-time simulations: Sensitivities

- gridded output from *backward-time simulations* is an *emission sensitivity*
- Which regions potentially influenced the receptor point?
- units: *seconds*
- *How long did air parcels arriving at the receptor spend in this grid cell in each step?*

Source contribution

- backward simulations can be used to calculate the *contribution of individual emission sources* to a measurement
- needed:
    - gridded sensitivities from the model output
    - data on emission fluxes (units: *mass* / *volume* / *second*)
        - wait, what — per *volume*?
- then: multiply sensitivities (in *seconds*) with emission fluxes
  $\rightarrow$ resulting units: *mass* / *volume* $\rightarrow$ the same units as a measurement!
- result: for each grid cell and time step:
  How much did emissions from there and then contribute to the measurement?
    - when summing this over the whole model domain and all time steps: total measurement

Source contribution (*black carbon* measurements during *EMeRGe-EU*)

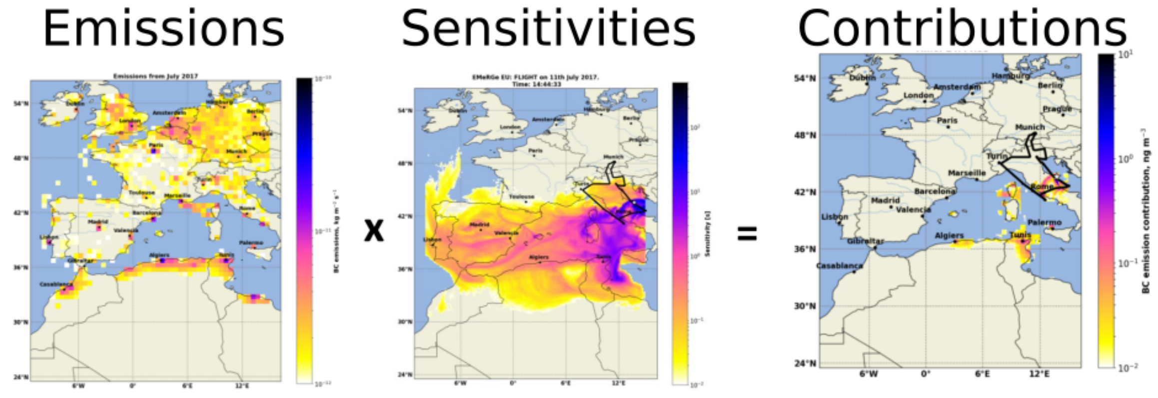

Figure 11: Principle of calculating source contributions (from A.B. Kalisz Hedegaard)

Loss processes

Loss processes in a Lagrangian model

- a Lagrangian model only simulates *transport* of air masses
- no interaction between air parcels
- but: loss processes *independent from all other air parcels* can be implemented:
  - radioactive decay
  - wet deposition / wash-out by rain and snow
  - dry deposition / sedimentation, impaction, …
  - chemical reaction with other species of known concentration
    - e.g., reaction of CH_4 with OH, using a global OH *climatology*

What does particle loss mean for the model output?

- e.g., rain leads to wash-out
- *forward* simulations:
    - after a plume passes through rain, the tracer *mass* in the affected air parcels is reduced
- *backward* simulations:
    - “after” a plume passes through rain, the *sensitivity* in the affected air parcels is reduced

Applications of Lagrangian models

A list of Lagrangian transport models

Some examples of Lagrangian transport models are:

- FLEXPART (developed by NILU, BOKU, ZAMW; see Stohl et al. 2005)
- HYSPLIT (developed by NOAA; possible to use via web-based interface; see Stein et al. 2015)
- NAME (developed by UKMO; see Jones et al. 2007)
- STILT (developed by UWaterloo, MPI-BCG, Harvard, . . .; see Lin 2003)

Dispersion of methane emissions in Upper Silesia (Poland)

- ~80 methane emission sources (coal mines) in small region
- *CoMet* campaign: methane measurements from an aircraft
- simulate transport to better understand measurements
- [link to movie]

Cesium-137 deposition after Fukushima (FLEXPART)

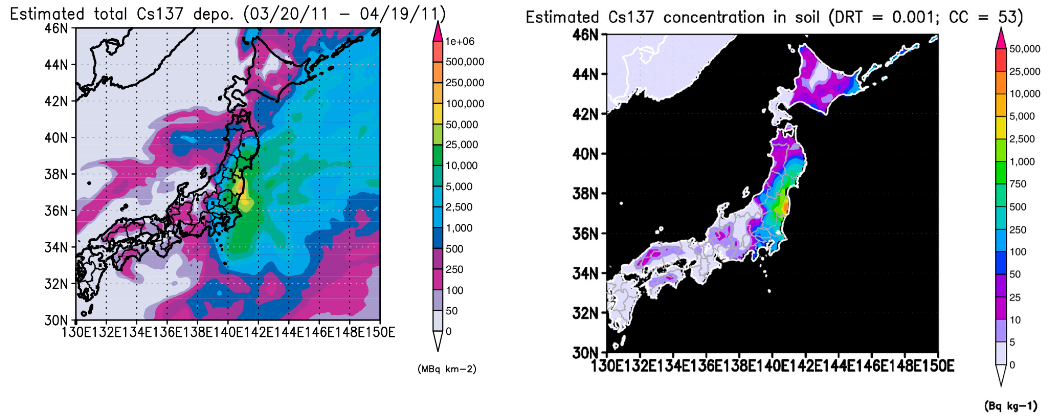

Figure 12: Cs-137 deposition (left) and soil concentration (right) after the Fukushima nuclear incident (from: Yasunari et al. 2011)

- Assume Cs-137 emissions from Fukushima nuclear accident
- Simulate transport, decay, deposition

- Results:
  - total Cs-137 deposition
  - Cs-137 concentration in soil

Influence of Siberian biomass burning on the Arctic (HYSPLIT)

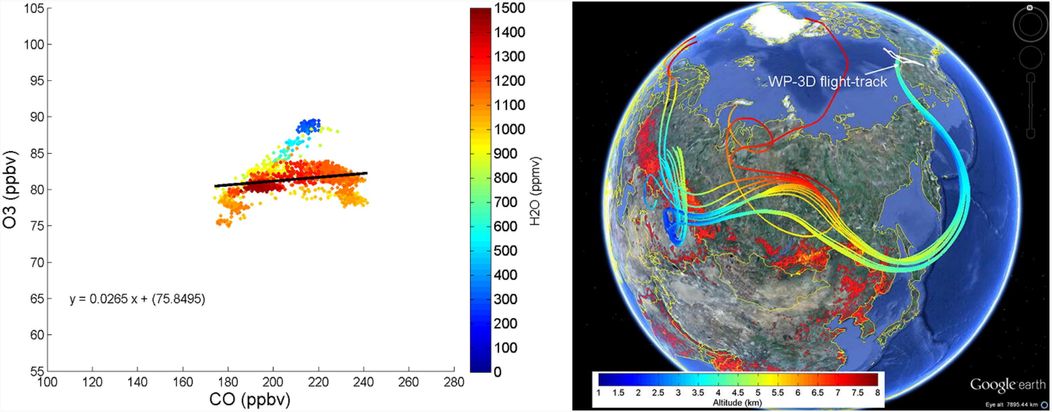

Figure 13: O_3 / CO ratio (left) and backward trajectories (right) from the ARCPAC campaign (from: Pommier et al. 2012)

- Measurements show two clearly distinguishable types of air
- Back-trajectories help identify source regions and explain the observations: high-CO air masses from Siberian forest fires

Emission sensitivities for deposited mass (FLEXPART)

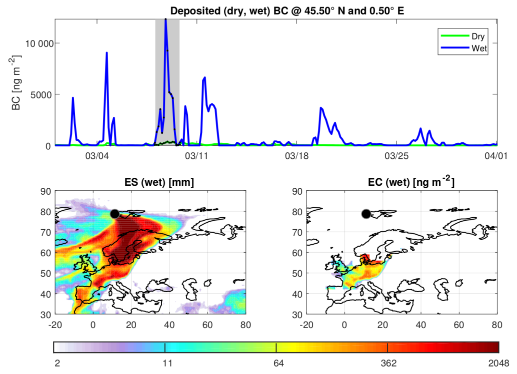

Figure 14: Emission sensitivity and contribution for deposited black carbon in Svalbard (from: Eckhardt et al. 2017)

- Observation of high BC wet deposition in Svalbard
- Backward simulation provides surf. layer *emission sensitivity*
- Multiplication with emission inventory (ng m^{-3} s^{-1})
- Contribution of source grid cells to meas. deposition

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