LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

FAKULTÄT FÜR PHYSIK
METEOROLOGIE

MIM

BEATBOX v1.0: Background Error Analysis Testbed with Box Models

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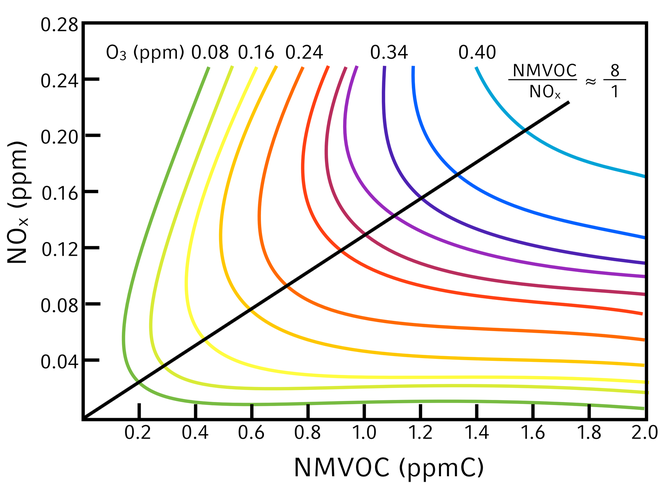
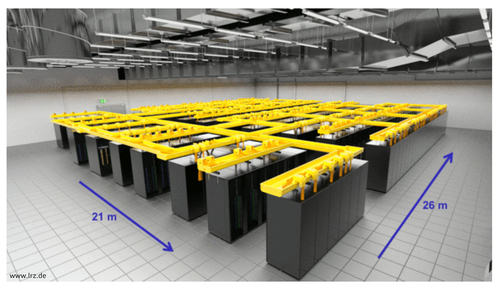
What happens to atmospheric chemistry when we assimilate data?



- highly non-linear system
- important species (e.g. O_3) not observed
- strongly resolution-dependent
  (urban centers: VOC-limited, suburbs: NO_x-limited)
- spatially and temporally variable

How can we investigate this?



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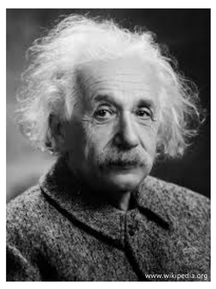
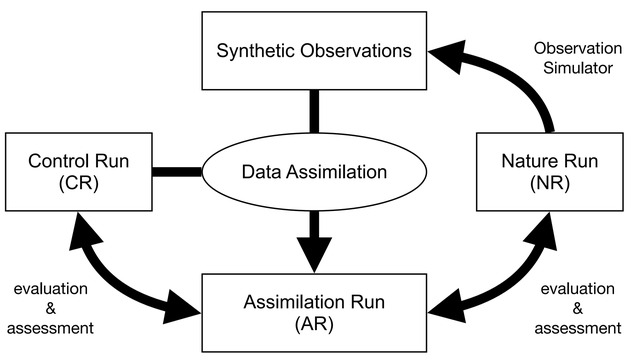


Realistic 3D models with chemical data assimilation are expensive (ensemble) and/or complicated (variational)

BEATBOX: data assimilation toy model using BOXMOX

(Knote et al., GMD, 2018)

python powered



- **O**bserving **S**ystem **S**imulation **E**xperiments
- Aircraft campaign data for test cases provided
- several DA methods included
  (ensemble, hybrid, variational)
- inflation, cycling, …

Configuration

```
[Global]
mech_nr = MCMv3_3
…

[genBOX]
perturbspecies = CH2O
rel_stdev_scaleic = 0.05
pert_distric = normal
…

[BOXMOX]
runtime = 3.0
dt = 180.0

[BEATBOX]
state = NO2, O3, CH2O, OH
obs = CH2O
…

[Cycling]
nfcst = 20
```

Simple text file.

Documentation

Box modeling code repository

A number of tools used for box modeling. All packages are avaible on PyPI, ins

```
pip install <package>
```

- beatboxtestbed (Background Error Analysis Testbed with Box Models)
- boxmox (Python wrapper for the chemical box model BOXMOX)
- chemspectranslator (Universal translator for chemical mechanism species
- frappedata (FRAPPE dataset connector for boxmox)

Available online.

Installation

```
> pip install beatboxtestbed
```

BEATBOX is a set of Python (v2) packages, available on Python Package Index (PyPI). BOXMOX is required.

Making a simulation

```
> make_BEATBOX_cycling_run CH2Oac settings_CH2Oac.cfg
```

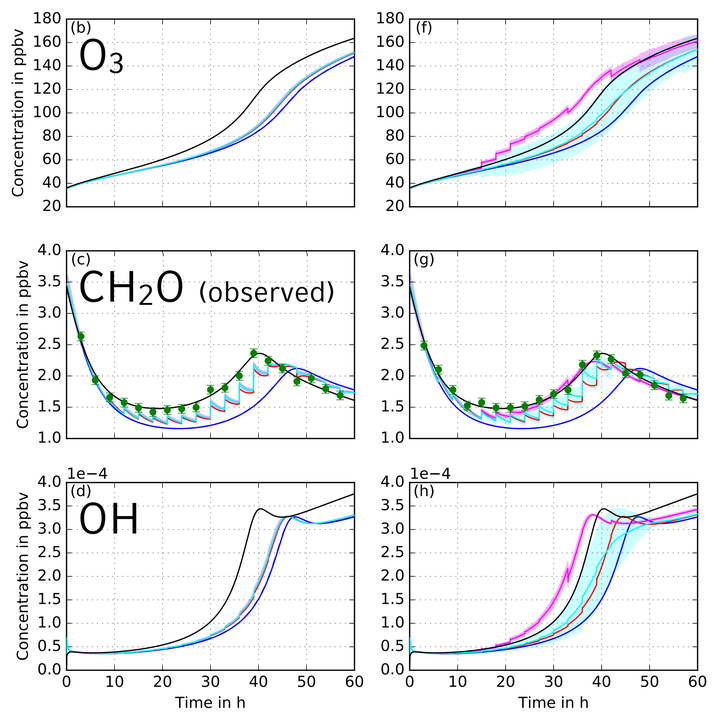
Settings defined in configuration file, conduct simulation with command line scripts. Parallelized execution through Python `joblib` package.

Plotting results

```
> archive_path = h.get_archive_path('CH2Oac')
> fig, ax = plt.subplots()
> fig = p.sensitivities(archive_path, fig)
> fig.savefig('sensitivities.png')
```

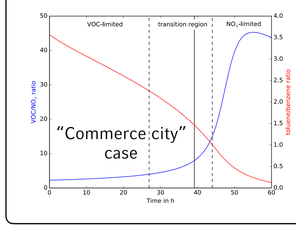
Python `matplotlib` plotting routines included.

Effects on the unobserved chemical state of the atmosphere



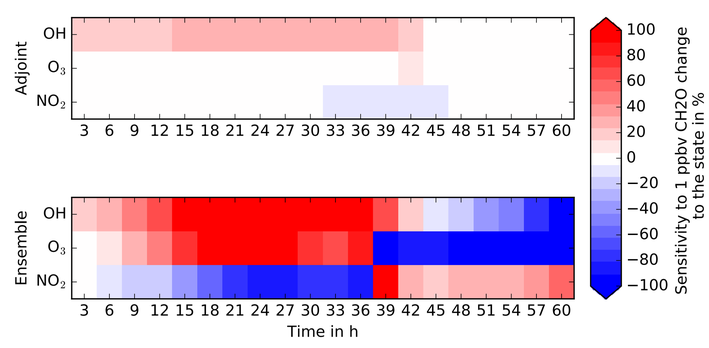
Test case

- photochemistry in a jar
- urban air mass sample



- chosen DA method strongly influence outcome
- sensitive to localisation
- effects vary with chemical regime
- assimilating NO_2 has no influence on rest of state vector
  (not shown)

Sensitivity analyses

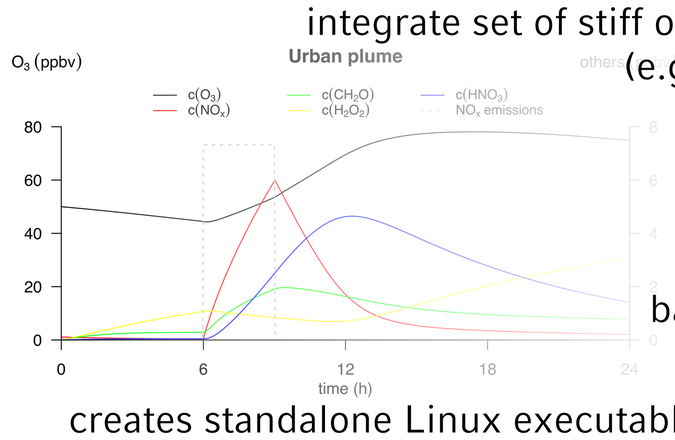


- sensitivity depends on selected DA method
- varies with chemical regime (over time)
- abrupt changes observed during regime transition

BOXMOX: tropospheric chemistry box model

(Knote et al., Atm. Env, 2015)

integrate set of stiff ordinary differential equations (e.g., photochemistry) over time



box model processes (emissions, dilution, …)

simple text file I/O

based on Kinetic PreProcessor (Damian et al., 2002)

creates standalone Linux executables, Python wrapper available

Conclusions

- Python-based data assimilation toy model developed
- OSSEs with different DA methods
- Test cases demonstrate insightful results
- Model freely available for the community
- Full documentation online

References

Damian, V., Sandu, A., Damian, M., Potra, F., and Carmichael, G.R. (2002). The Kinetic PreProcessor KPP -- A Software Environment for Solving Chemical Kinetics, Computers and Chemical Engineering, Vol. 26, No. 11, p. 1567-1579.

Knote, C., Tuccella, P., Curci, G., Emmons, L., Orlando, J. J., Madronich, S., … and Forkel, R. (2015). Influence of the choice of gas-phase mechanism on predictions of key gaseous pollutants during the AQMEII phase-2 intercomparison. Atmospheric Environment, 115, 553-568.

Knote, C., Barré, J., & Eckl, M. (2018). BEATBOX v1. 0: Background Error Analysis Testbed with Box Models. Geoscientific Model Development, 11(2), 561-573.

https://boxmodeling.meteo.physik.uni-muenchen.de