CAMxRunner: A modular environment for efficient CAMx simulations

Daniel C. Oderbolz (daniel.oderbolz@psi.ch), Şebnem Andreani-Aksoyoğlu, Johannes Keller, Iakovos Barmpadimos, André S.H. Prévôt

Laboratory of Atmospheric Chemistry (LAC), Paul Scherrer Institut, Switzerland

PAUL SCHERRER INSTITUT

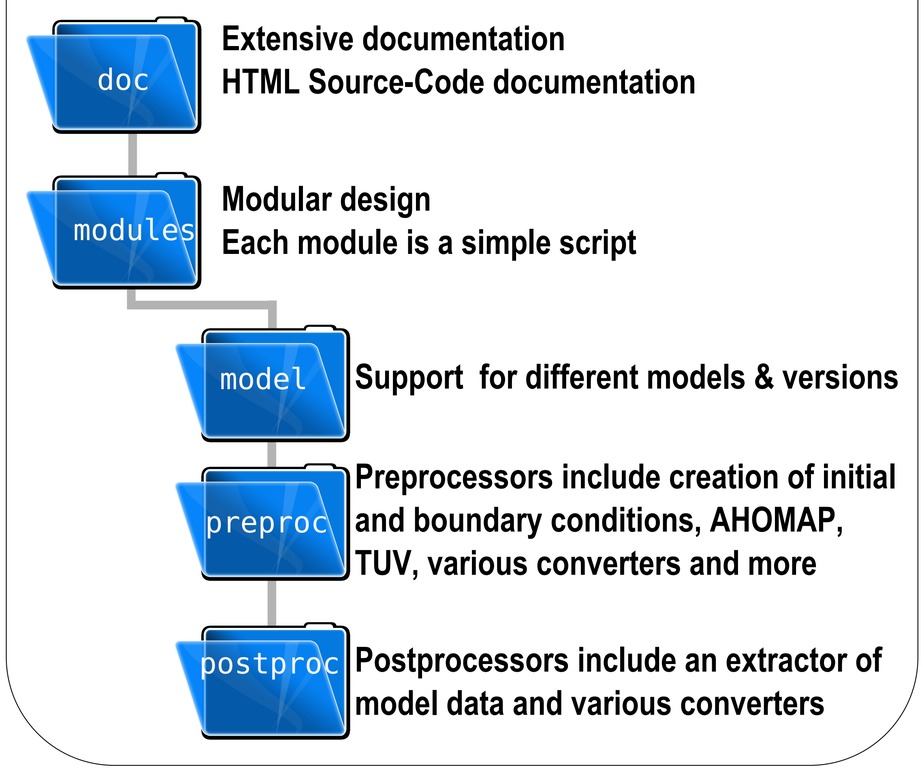
Goals

- **Eliminate human errors in the use of air quality models**
- **Enhance reproducibility**
- **Increase modelling speed**
- **Enable use of different model versions**
- **Save disk-space**

The system

- is written in the shell language Bash
- stores configuration data centrally
- saves time by parallel execution (see right)
- is modular, so that all pre- and postproc. in our lab could be integrated
- saves space by dynamic compression
- separates models using a clean structure
- helps the user to compile source codes

Features & Structure (excerpt)



Acknowlegements

- Partly funded by the Swiss Federal Office for the Environment (FOEN)
- CAMx is provided by ENVIRON Inc. (free)
- Icons: px+mx, Double J Design

Using CAMxRunner

- The installer guides the user through setup & compilation of source code
- CAMxRunner can be adapted to most environments by configuration
- The system can be adapted to virtually any naming convention by rules:

Bash Variable

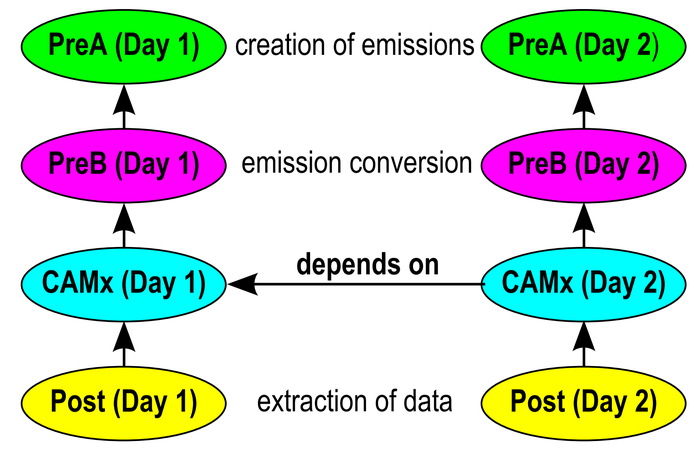
```
CXR_PHOTOLYIS_RATES_FILE_RULE='${CXR_INPUT_DIR}/tuv_${CXR_YEAR}_${CXR_WOY}.out'
```

At runtime is resolved to `/my_input_dir/tuv_2006_51.out'`

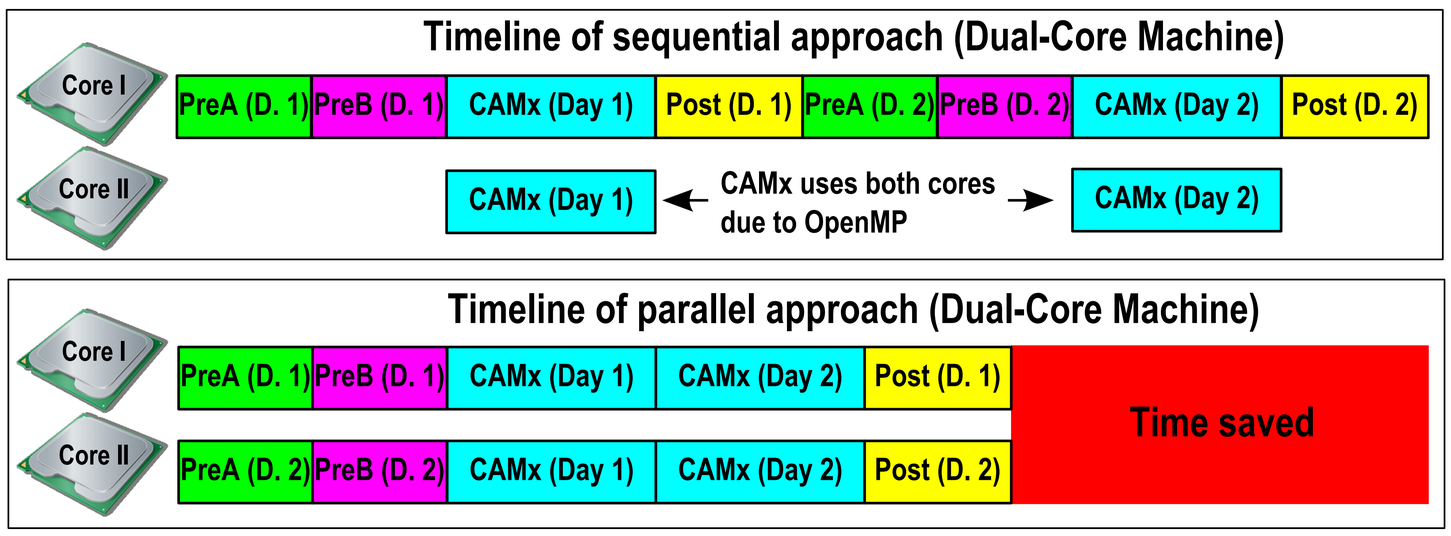
- Often-used settings can be stored in a "base-configuration"
- Before an actual run, a so-called dryrun detects configuration issues
- At runtime, the system can notify the user of errors by Email/SMS/Twitter

How does Parallelization work in CAMxRunner?

- Sorting steps according to dependencies
  Example: simple 2-day run (arrows indicate dependencies)

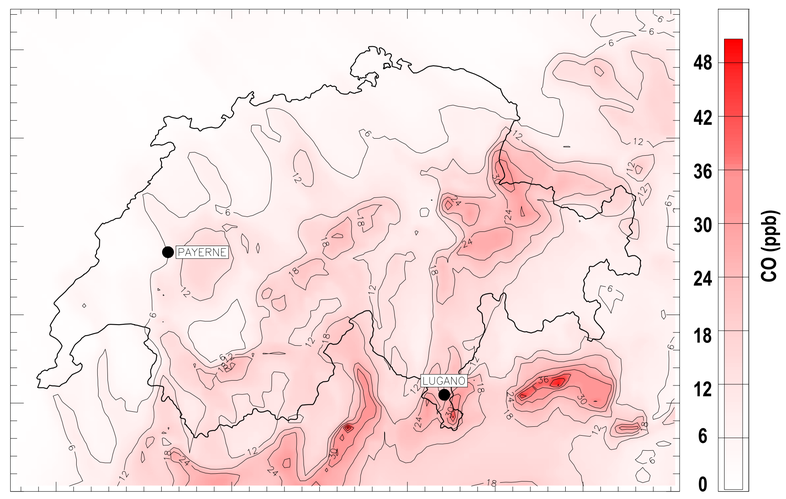


- Execution of the plan in parallel (by background processes)
- Before starting a step, its dependencies are checked



Compiler flags may influence outcome of a simulation

- Both runs used CAMx 4.51
  A was compiled with PGI
  B with Intel
- Difference diminishes when `-fltconsistency` flag of Intel compiler is active
- That is why CAMxRunner stores the compiler flags used!



Difference A-B of CO after 14 model hours (56 steps) with CAMx 4.51
A: Model compiled with pgf90 7.1.1. B: Model compiled with ifort 11.1