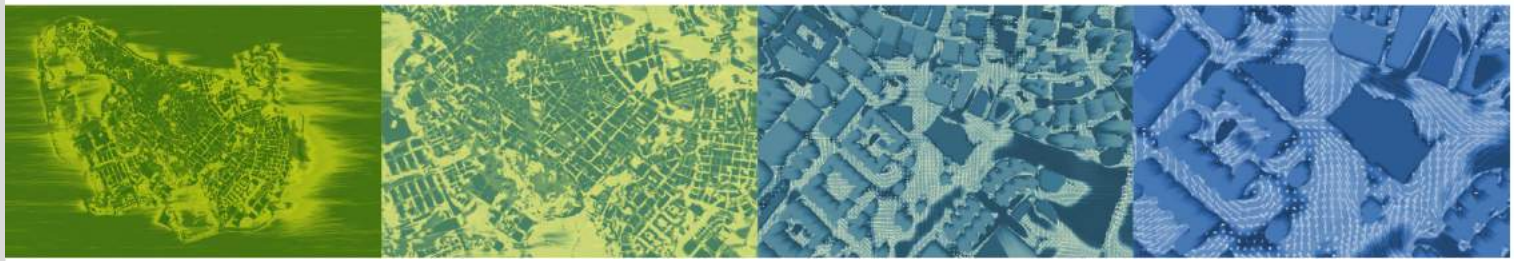
[UC]² Urban Climate Under Change
Stadtklima im Wandel

SPONSORED BY THE
Federal Ministry of Education and Research

Development of an online chemistry modele for the microscale urban climate model PALM-4U within the [UC]² programme

Sabine Banzhaf[1], R Forkel[2], B Khan[2], M Kurppa[15], E Chan[1], E Russo[1], M Schaap[1], M Mauder[2], K Ketelsen[3], B Maronga[4], S Raasch[4], F Kanani-Sühring[4], M Sühring[4]
and: M Belda[14], B Büter[12], T Esch[5], D Fröhlich[6], T Gronemeier[4], G Groß[4], W Heldens[5], A Hellsten[11], T Lang[7], E Kadasch[6], P Krč[13], H Maamari[9], A Matzarakis[6], G Meusel[4], M Pallasch[9], D Pavlik[12], J Pfaferott[7], J Resler[13], S Rißmann[7], MH Salim[10], C Schneider[10], M Schrempf[4], S Schubert[10], G Seckmeyer[4], H Sieker[9], RH von Tils[4], S Ward[4], K Winderlich[6] und J Zeidler[4]

1 Freie Universität Berlin | 2 Karlsruher Institut für Technologie | 3 Software Consultant | 4 Leibniz Universität Hannover | 5 Deutsches Zentrum für Luft- und Raumfahrt | 6 Deutscher Wetterdienst | 7 Hochschule Offenburg | 9 Ingenieurgesellschaft Prof. Dr. Sieker mbH | 10 Humboldt-Universität zu Berlin | 11 Finnish Meteorological Institute | 12 GEO-NET Umweltconsulting GmbH | 13 Czech Academy of Sciences, Czech Republic | 14 Charles University, Prague, Czech Republic | 15 University of Helsinki

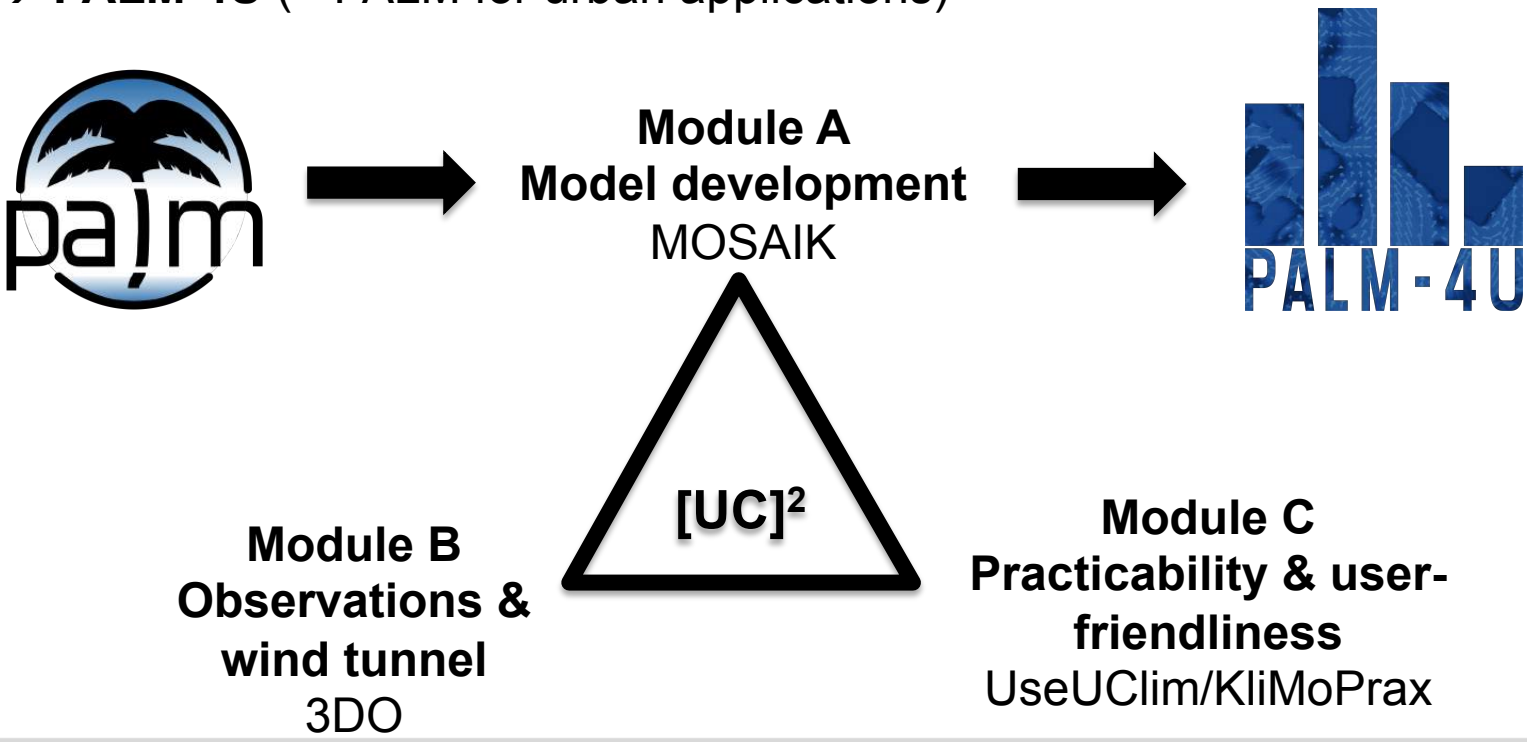


MOSAIK

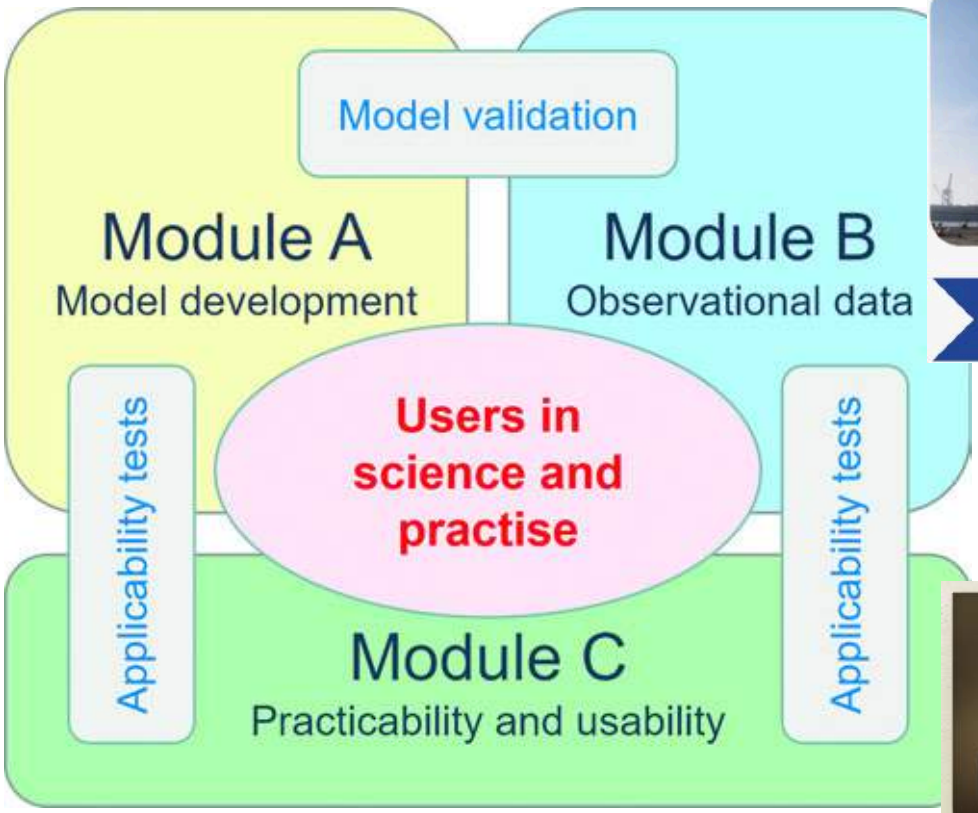
[UC]²: Project structure

- **Urban Climate Under Change [UC]²:** Research project funded by the German Federal Ministry of Education and Research (BMBF), 2016-2019

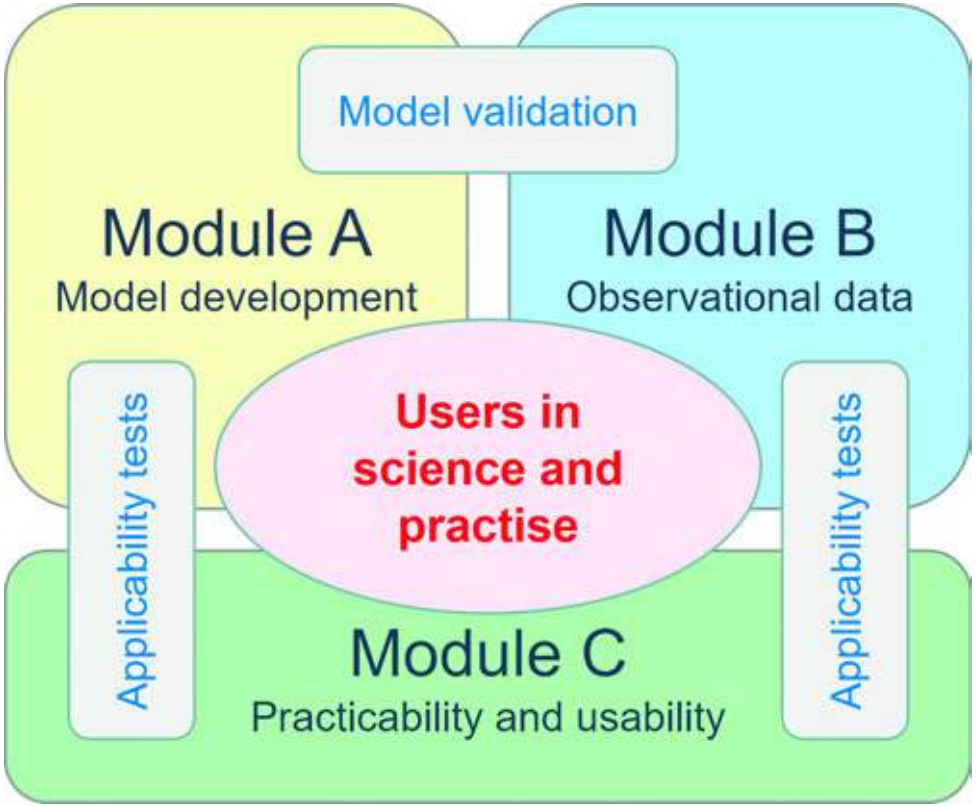
- **Goal:** Development of a new (building resolving) urban climate model for scientific research and applied urban planning
  → **PALM-4U** (= PALM for urban applications)



[UC]^2: Project structure



[UC]²: Project structure



[UC]² Publications

Scherer et al., 2019: *Urban Climate Under Change [UC]² – A National Research Programme for Developing a Building-Resolving Atmospheric Model for Entire City Regions*
DOI: 10.1127/metz/2019/0913

Maronga et al., 2019: *Development of a new urban climate model based on the model PALM – Project overview, planned work, and first achievements*
DOI: 10.1127/metz/2019/0909

Scherer et al., 2019: *Three-Dimensional Observation of Atmospheric Processes in Cities*
DOI: 10.1127/metz/2019/0911

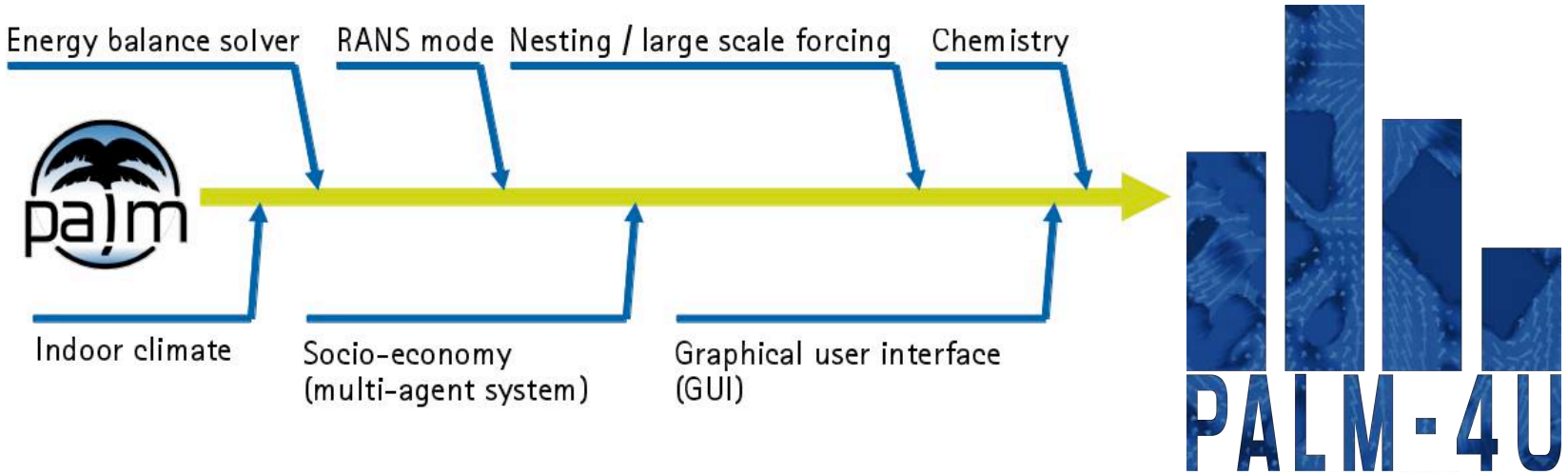
Halbig et al., 2019: *Urban Climate Under Change – Module C of the Research Programme: User Requirements and Case Studies to Evaluate the Practicability and Usability of the Urban Climate Model PALM-4U.*

Module A: From PALM to PALM-4U
Overview of capabilities

PALM: the model core (Maronga et al. 2015, GMD)

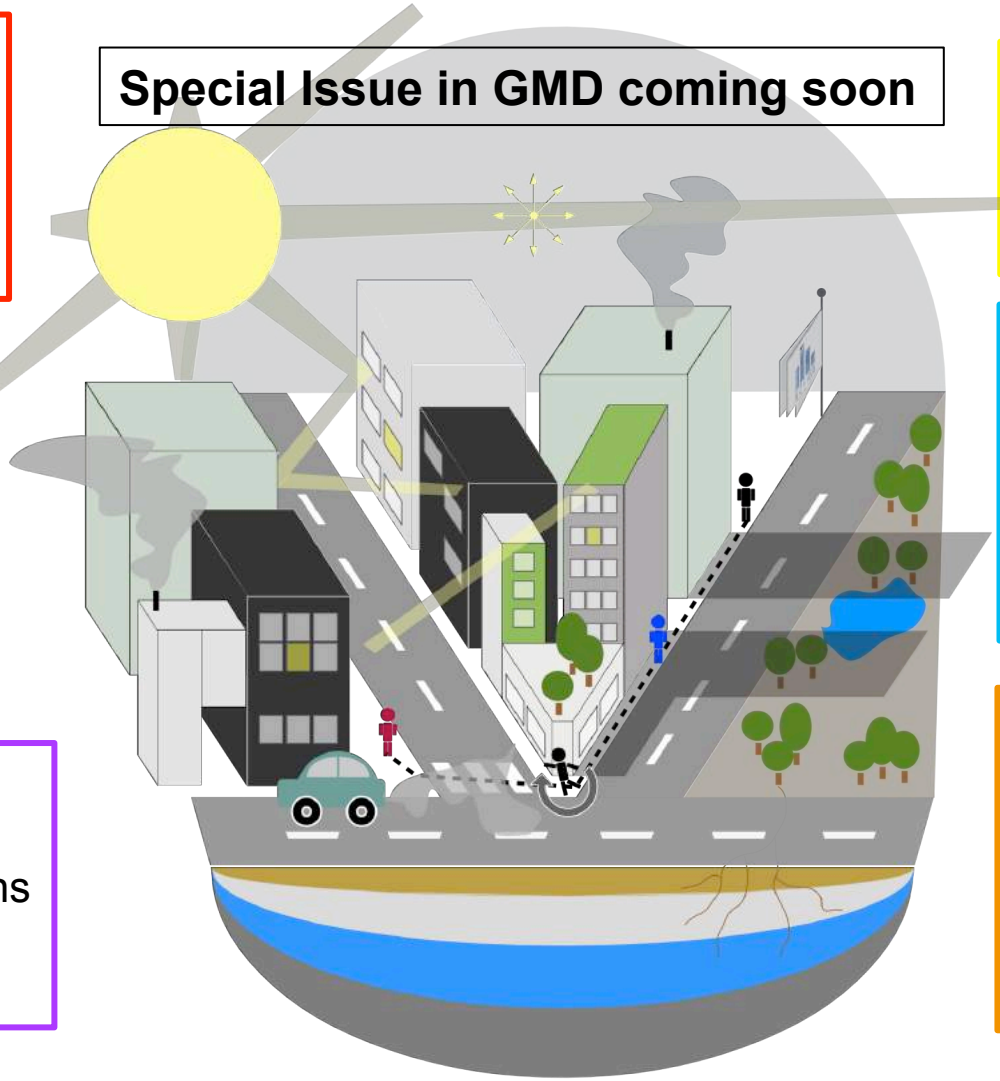
- Parellelized large-eddy simulation (LES) model
- Incompressible and anelastic
- Highly-optimized, high scalability
- Topography on Cartesian grid
- Embedded models

PALM-4U: PALM + additional components



Processes in PALM-4U

Special Issue in GMD coming soon



Urban Surfaces
- Energy balance
- Heat conduction
- Solid materials
- Green elements

Vegetation
- Energy balance
- Sink for momentum
- Shading
- Roots
- Soil moisture

Chemistry
- Transport
- Chemical reactions
- Photolysis
- Emissions

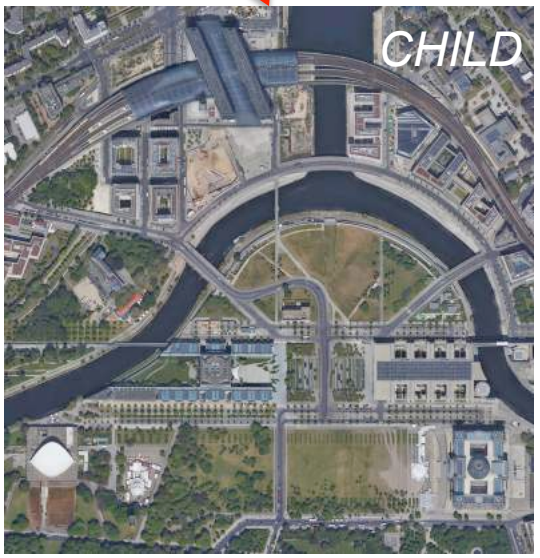
Radiation
- Energy balance
- Shading
- Reflections

Impact
- Multi-agent system
- Biometeorological analysis
- Indoor climate

Technical Solutions
- Mesocale nesting
- LES-LES nesting
- RANS mode
- User-friendly GUI

Berlin showcase: Set-up

- 24h simulation (21/7/13), Start 0:00 MESZ
- 24h spinup: Surface and radiation
- *„parent“* domain:
  Berlin (47 x 39 km^2 @ 10m resolution)
- *„child“* domain:
  Government district (1 km^2 @ 1m res.)
- Forcing: COSMO-DE initial profiles, 21 July 2013 at midnight
- Synoptic situation: weak winds, clear sky, COSMO-DE near-surface temperatures of > 303 K
- Lateral boundaries: (from parent) cyclic

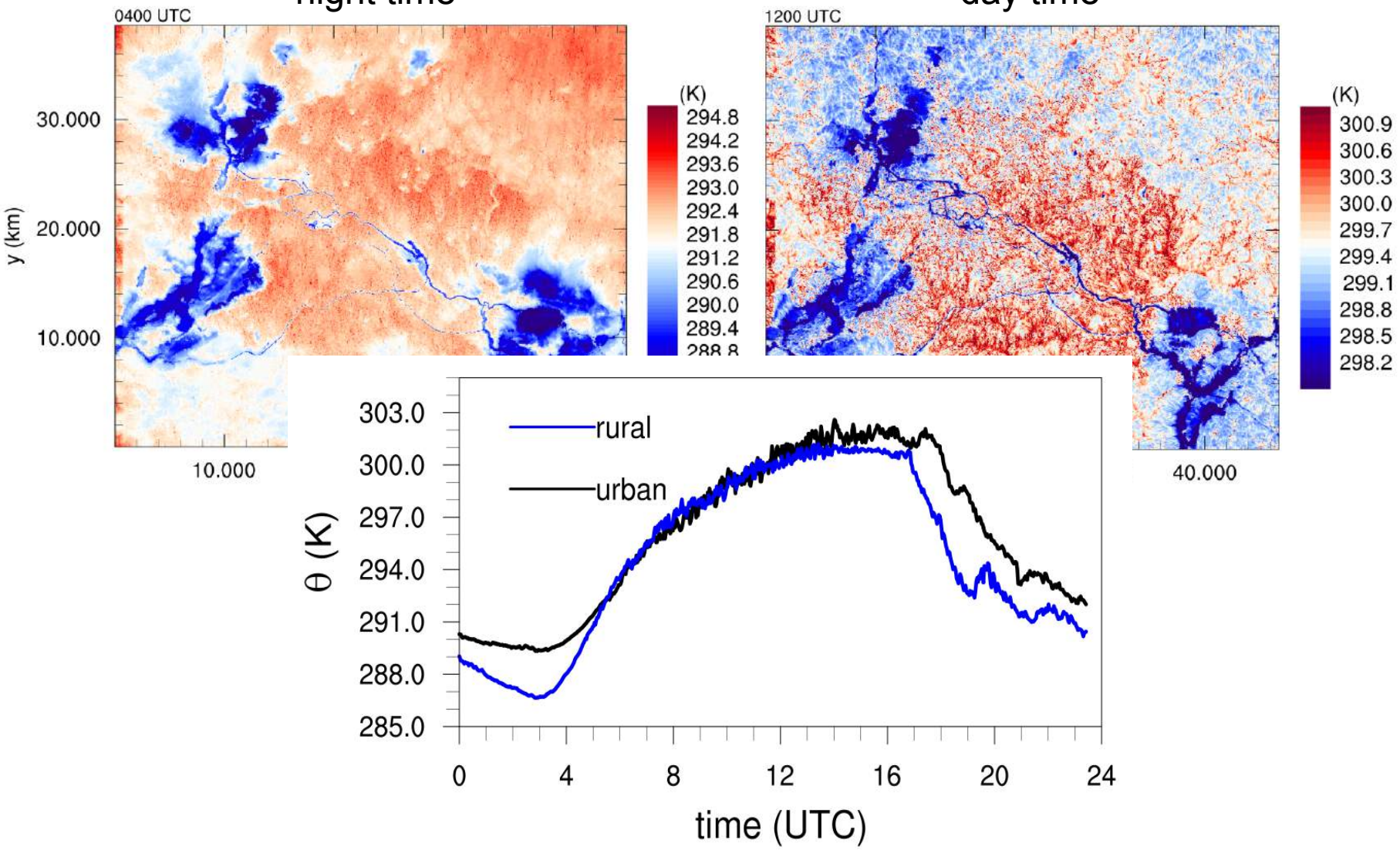


Resources:
parent:
4704*3920*336 grid points, 10.976 cores, 11 Tbyte memory
child:
1024*1024*320 grid points, 1.024 cores
1h real time ~ 15 h wall clock time

Berlin showcase: Air temperature

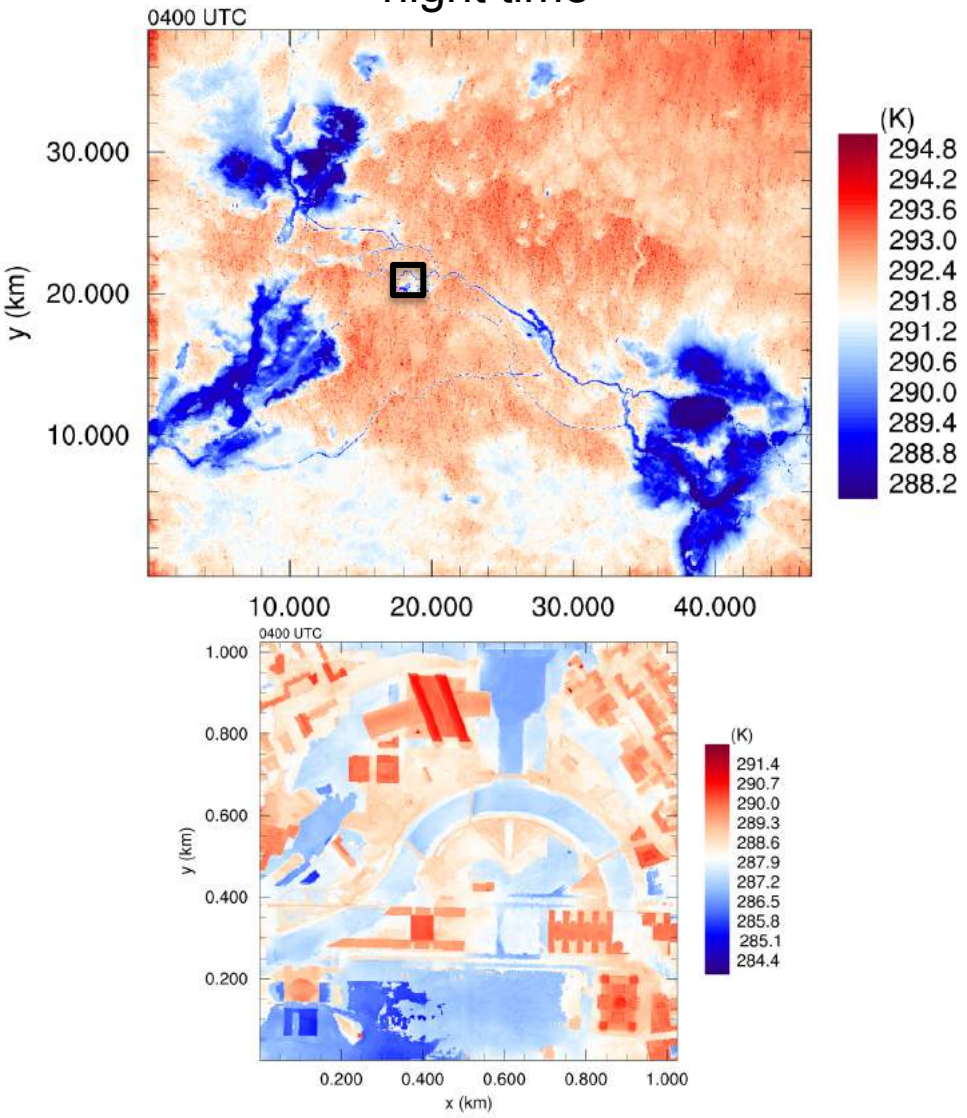
night time

day time

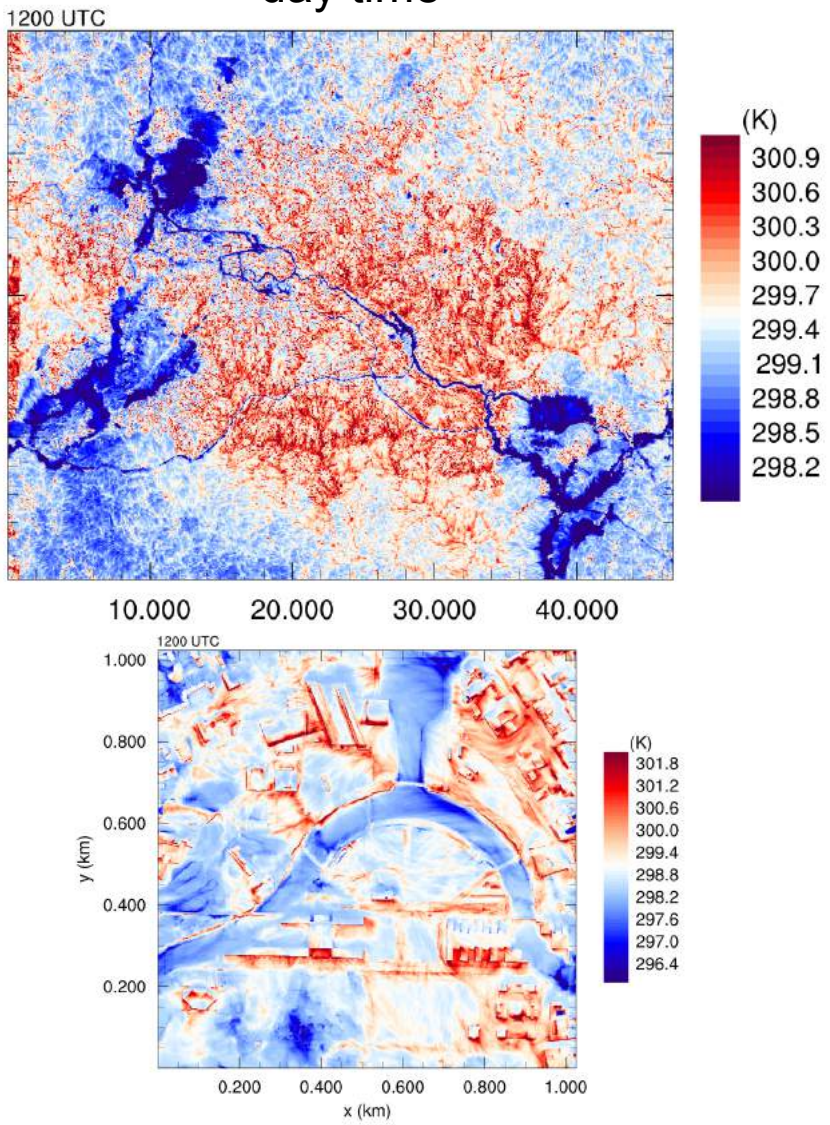


Berlin showcase: Air temperature

night time



day time



Chemistry module (1)

- An 'online' chemistry model has been implemented into PALM-4U
- Gasphase chemistry
  - Automatic generation of chemistry code with the **K**inetic **P**re-**P**rocessor (KPP, Damian et al., 2002) allows for high flexibility in the choice of gas phase chemical mechanisms
  - Adaption for PALM-4U based on KP4 post-processor (Jöckel et al., 2010)
  - PALM-4U includes a set of chemistry mechanisms of different complexity

→ Complexity of mechanism chosen by user depending on application

→ Mechanisms can easily be added by user

Chemistry module (2)

CBM4: Carbon Bond Mechanism (Gery et al. 1989, 32 compounds, 81 reactions)

SMOG: Small photochemical mechanism (13 compounds, 12 reactions)

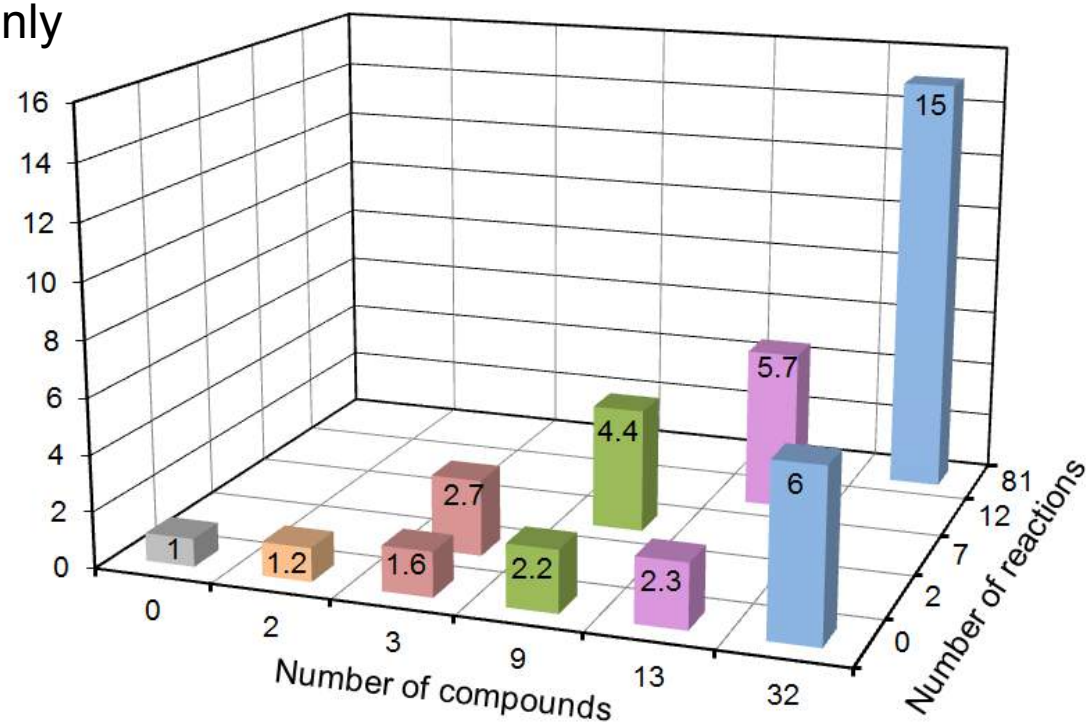
SIMPLE: Simplified of SMOG (9 compounds, 7 reactions)

PHSTAT: Photo-stationary state (3 compounds, 2 reactions)

PASSIVE: Two passive tracers (2 compounds, 0 reactions)

Reference: Meteorology only

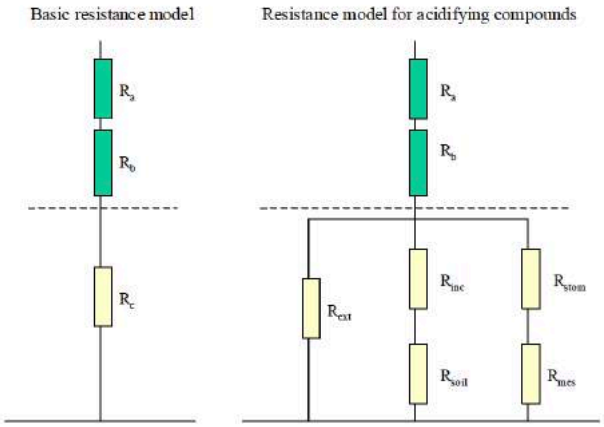
Resources:
PALM-4U chemistry run using the different provided mechanisms



Chemistry module (3)

- A simple photolysis parameterization: Dependency on solar altitude and chemical component following Saunders et al. (2003)

- Try deposition following resistance approach
  - DEPAC module for gases (van Zanten et al., 2010)
  - Reactive and passive aerosols following Zhang et al. (2001)



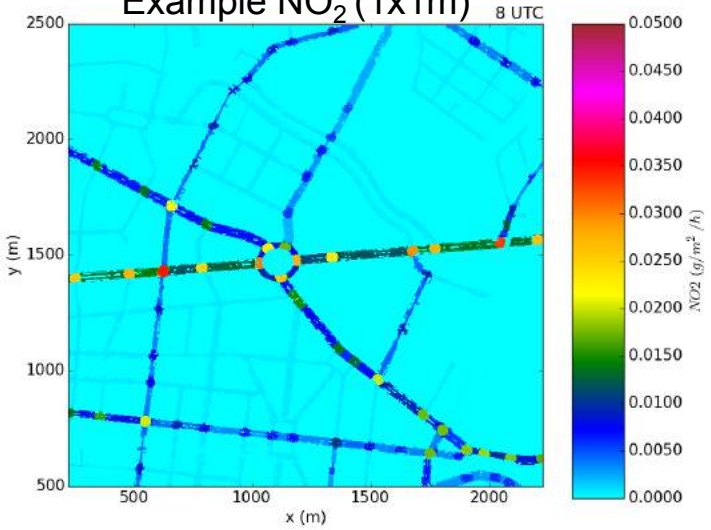
- Coupled to the sectional aerosol module SALSA (Kokkola et al., 2008) which has been implemented into PALM
  → External contribution, Kurppa et al. 2019 (GMD)

Chemistry module (4)

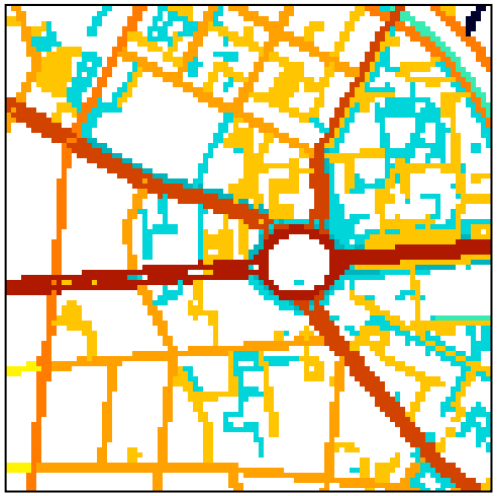
- Emission module:
  Anthropogenic emissions can be provided in different levels of detail

(1) Via netcdf input as gridded data, temporally disaggregated or annual emission informatior

Example NO_2 (1x1m)



Street type (10x10m)

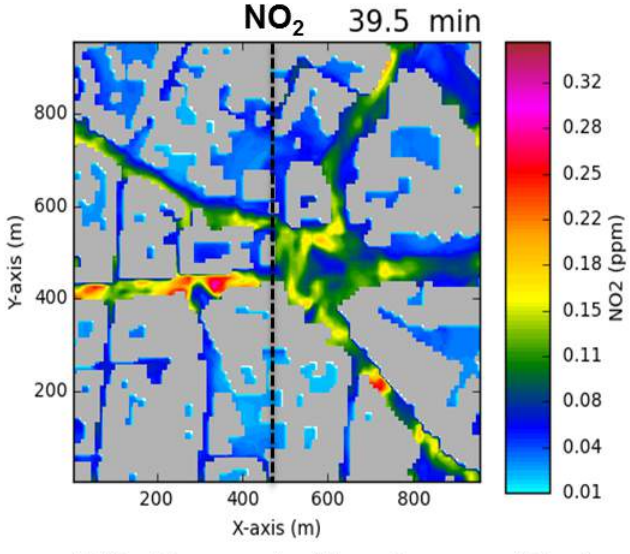


main road
side road
other

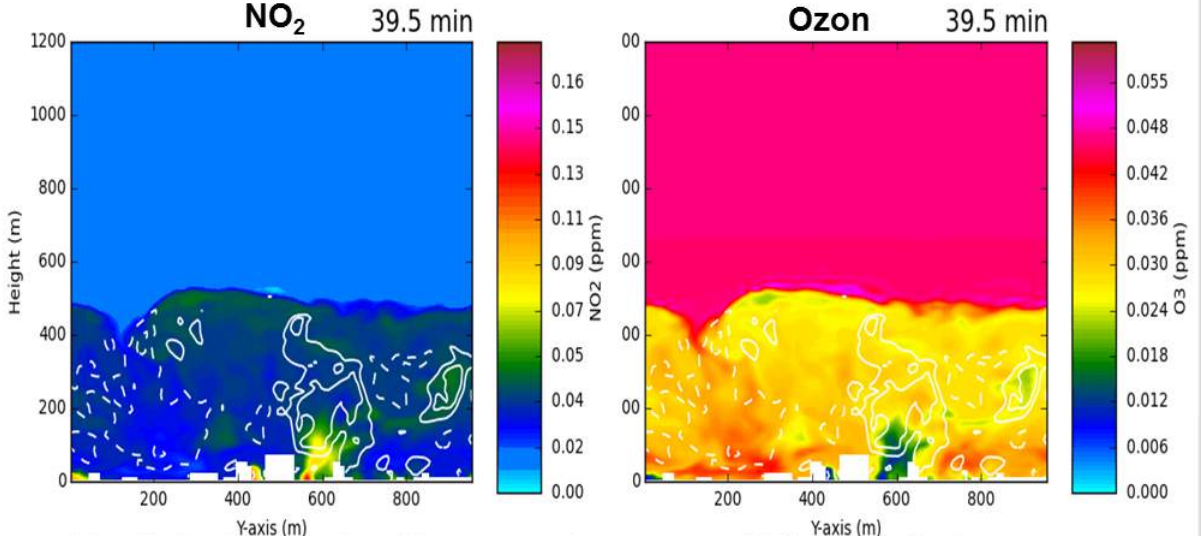
(2) Parameterised traffic emissions relying on the street type classes from OpenStreetMap and emission factors following HBEFA 3.3, input via namelist

Chemistry module – First results

- Berlin, Germany, Ernst-Reuter-Platz
- 10 m resolution, 1km x 1km x 3 km
- Parameterised traffic emissions relying on street type
- Small photochemical mechanism ‘SMOG’ (13 compounds, 12 reactions)
- Summer time simulation, 21st of July



Concentration of NO_2 in ppm (5m)



Z-Y-vertical cross section at dashed line : Concentration (shaded color) of NO_2 and O_3 in ppm and vertical velocity (-2.0 to 2.0 m s^{-1}, negative values as dashed lines)

Chemistry module – First results

- Berlin, Germany, Ernst-Reuter-Platz
- 10 m resolution, 1km x 1km x 3 km
- Parameterised traffic emissions relying on street type
- Small photochemical mechanism ‘SMOG’ (13 compounds, 12 reactions)
- Summer time simulation, 21st of July

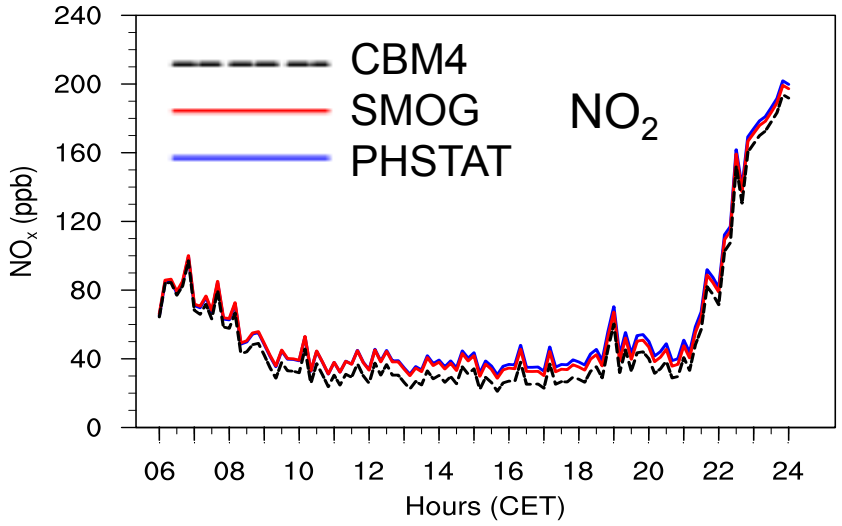
Animation!!!

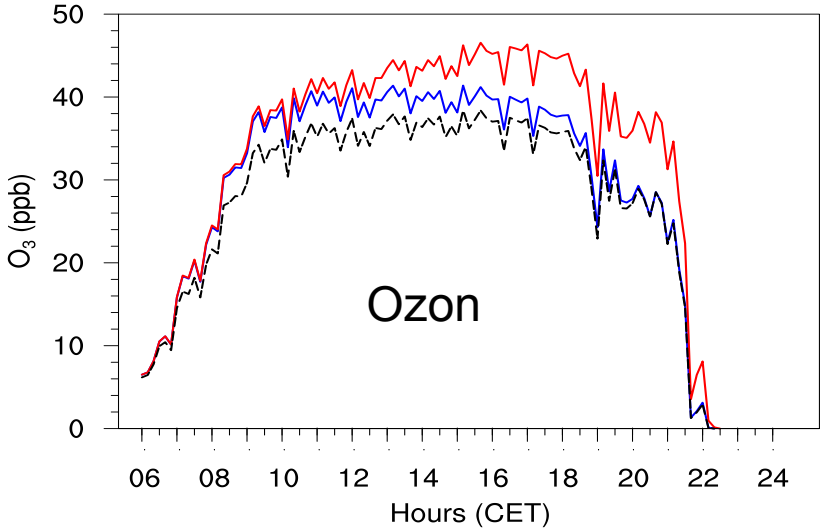
Concentration of NO_2 in ppm (5m)

Z-Y-vertical cross section at dashed line : Concentration (shaded color) of NO_2 and O_3 in ppm and vertical velocity (-2.0 to 2.0 m s^{-1}, negative values as dashed lines)

Chemistry module – First results

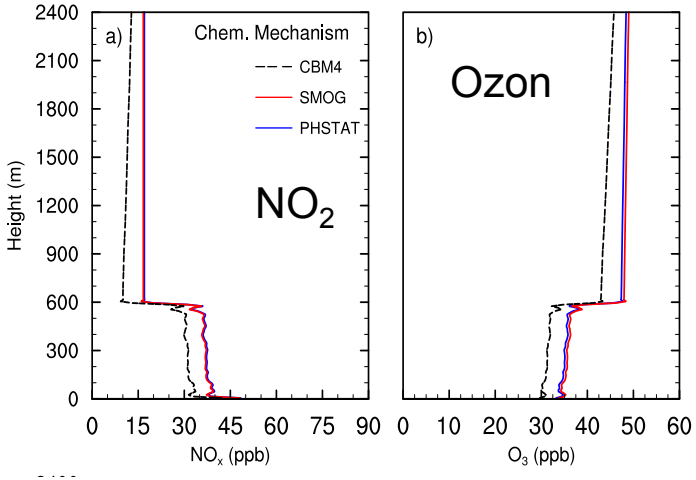
Diurnal cycle



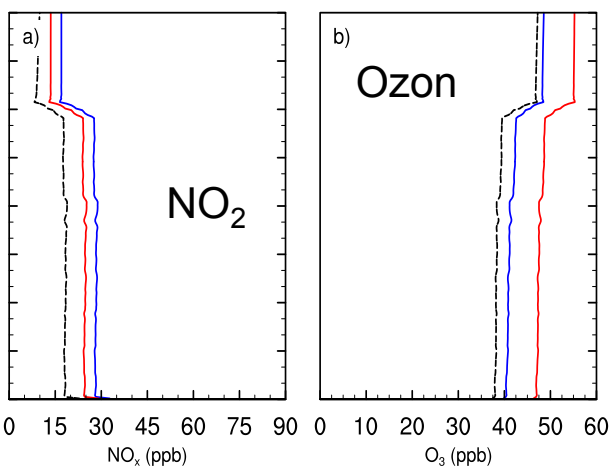


Profiles

09:00 CET

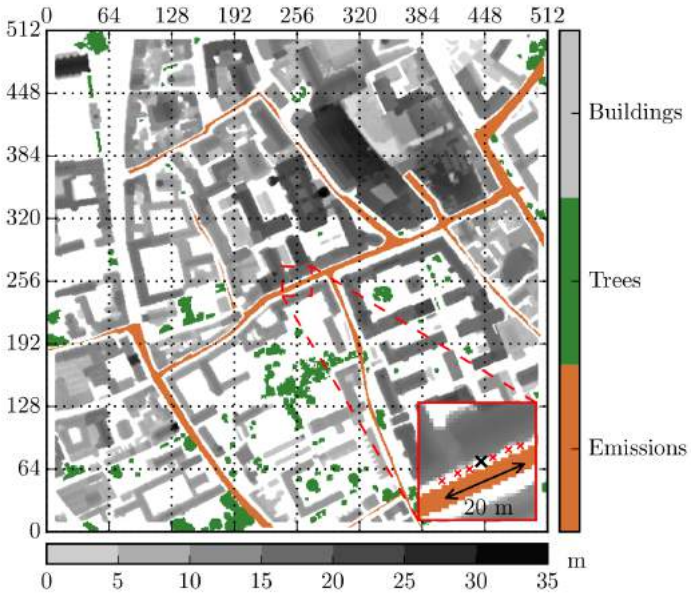


17:00 CET



Recognise the urban quarter below?

- Aerosol module SALSA coupled to PALM
- Implementation of SALSA and evaluation for a street-canyon (Pembroke Street) in central Cambridge
  → Kurppa et al., 2019 (GMD)
- 24 hours simulation @ 1m resolution on March 20–21, 2007 compared to measurements (Kumar et al., 2008, 2009)
- Parameterised emissions



Total aerosol number concentration Ntot (m^{-3})

Animation!!!

Conclusions and Outlook

- Turbulence and building resolving LES model including chemistry, applicable for scales way beyond street canyon, up to city-scale

- PALM-4U → Future state-of-the-art urban climate model

- Further improvements and applications of chemistry module
  - Comparison to measurements, city-scale applications
  - Connection to multi agent module → pollutant exposure
  - Offline Nesting: Lateral boundary conditions from mesoscale atmospheric chemistry model
  - Inclusion of pollen
  - Enhanced aerosol description
  - Biogenic emissions
  - Parameterised emissions for emissions from residential heating and large point sources
  - Wet deposition

Thank you for your attention!

sabine.banzhaf@met.fu-berlin.de

http://palm4u.org

https://palm.muk.uni-hannover.de/mosaik/wiki

http://palm-model.org

MOSAIK team + external partners

Leibniz Universität Hannover

Björn Maronga
Günter Groß
Siegfried Raasch
Gunther Seckmeyer
Farah Kanani-Sühring
Matthias Sühring
Tobias Gronemeier
Simon Ward
Robert von Tils
Michael Schrempf
Viola Weniger

Freie Universität Berlin

Sabine Banzhaf
Martijn Schaap
Emmanuele Russo

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

(Offenbach)
Kristina Trusilova
Eckhard Kadasch

(Freiburg)
Andreas Matzarakis
Dominik Fröhlich

GEO-NET

Dirk Pavlik
Björn Büter
Gregor Meusel

Klaus Ketelsen
(Software Consultant)

KIT Karlsruher Institut für Technologie

Renate Forkel
Matthias Mauder
Basit Khan

DLR Deutsches Zentrum für Luft- und Raumfahrt

Wieke Heldens
Thomas Esch
Julian Zeidler

Hochschule Offenburg
offenburg.university

Jens Pfafferott
Tobias Lang

HUMBOLDT-UNIVERSITÄT ZU BERLIN

Sebastian Schubert
Christoph Schneider
Mohamed Salim

Sieker
Die Regenwasserexperten

Matthias Pallasch
Heiko Sieker
Halim Maamari

CTU Czech Technical University in Prague

INSTITUTE OF COMPUTER SCIENCE
The Czech Academy of Sciences

Jaroslav Resler
Pavel Krc
et al.

FINNISH METEOROLOGICAL INSTITUTE

Antti Hellsten

HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

Mona Kurppa
Leena Järvi