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# First Results of Urban Microscale Air Quality Simulations for Berlin, Germany, Using PALM-4U

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# OUTLINE

### Background

- The MOSAIK Project
- PALM, The LES Model
- PALM-4U Components

### **Chemistry in PALM-4U**

- Interface between Chemistry and PALM-4U
- Current Features

### A Case Study from Downtown Belin-Germany

- Model Setup
- Simulation Domain
- Results

# **Summary and Outlook**









# BACKGROUND

# **The MOSAIK Project**

"Model-based city planning and application in climate change" (MOSAIK) to develop an urban climate model within the framework of Urban Climate Under Change ([UC]<sup>2</sup>).

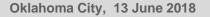
### 🗆 Main Aim

To develop a highly-efficient, state-of-the-art high-resolution microscale urban climate model that allows for building and turbulence-resolving simulations of large cities.

### **PALM**, the core Model

PALM (Reasch and Schröter, 2001; Maronga et al., 2015) was selected as the core model for the new microscale urban climate model named as PALM-4U of large cities such as Berlin (Germany).











# PALM, The LES Model.

- The PALM is based on the non-hydrostatic, filtered, incompressible Navier-Stokes equations in Boussinesqapproximated form.
- The Model has 6 prognostic quantities (u, v, w,  $\theta$ ,  $q_v$  and an optional 's' for passive tracer).
- An additional equation for subgrid scale TKE 'e' (default LES mode)

#### OR

the total TKE for Reynolds Averaged Navier-Stokes (RANS) mode.





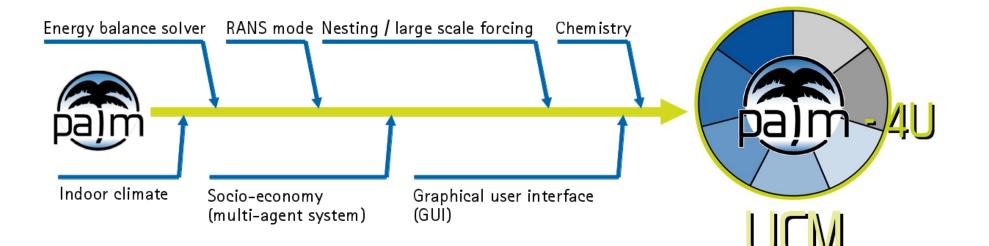






[Background]

#### • PALM-4U = PALM + Urban Climatology + Air Chemistry











# **CHEMISTRY IN PALM-4U**



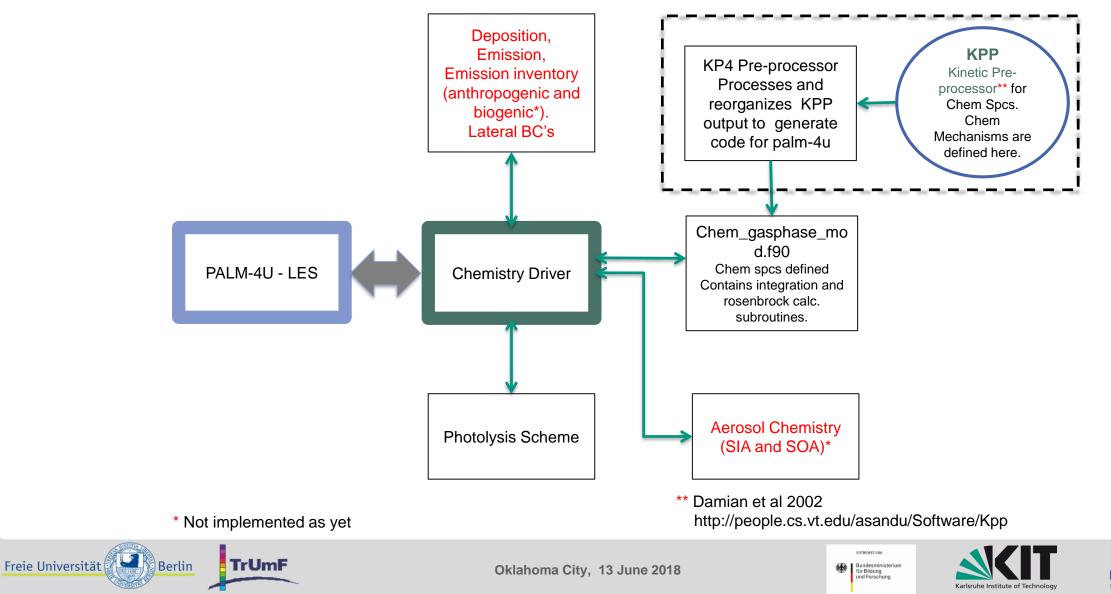






# **Interface b/w Chemistry and PALM-4U**

[Chemistry in PALM-4U]





# **Current Features**

### Current Features of Chemistry Model in PALM-4U Modeling System:

- An 'Online' coupled chemistry in LES mode for Gas-phase chemistry
- Chemical reactions
- Advection and diffusion
- $\circ$  **Photolysis**
- **o** Ability to take any user provided chemical mechanism
- Passive tracer
- $\circ$  Nesting
- $\,\circ\,\,$  Static emissions in time and space.









# A Case Study from Downtown Berlin - Germany

#### Model Setup

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- $\circ$  nX = nY = 96, nZ = 120; dX=dY=dZ =10 m; Ug = Vg = 1.0 m s<sup>-1</sup>
- Day & Time: 21 July, 5:00 UTC; Simulation length = 16 hours.
- Modules: radiation, urban surface model, land surface model,

canopy model, chemistry model, photolysis model

- Emissions related to OpenStreetmap street types: Enhancement factor for main roads = 1.667, Reduction factor for side roads = 0.334
- Emission: NO= 1.318 ppm s<sup>-1</sup>;NO<sub>2</sub>= 0.368 ppm s<sup>-1</sup>; RH=0.1804 ppm s<sup>-1</sup>; PM10 = 0.75 ug m<sup>2</sup> s<sup>-1</sup>.

#### The mechanism has 11 gas-phase chemical species and one non-reactive aerosol(PM10).

| $\{1.\}$ NO2 + hv = NO + O3          | : phot(j_no2)                        |
|--------------------------------------|--------------------------------------|
| $\{2.\}$ O3 + hv = 2OH + O2          | : phot(j_031d)                       |
| $\{3.\}$ NO + O3 = NO2               | : arr2( 1.8E-12_dp, 1370.0_dp, temp) |
| $\{4.\}$ RH + OH = RO2 + H2O         | : arr2( 2.E-11_dp, 500.0_dp, temp)   |
| $\{5.\}$ RO2 + NO = NO2 + RCHO + HO2 | : arr2( 4.2E-12_dp, -180.0_dp, temp) |
| $\{6.\}$ HO2 + NO = NO2 + OH         | : arr2( 3.7E-12_dp, -240.0_dp, temp) |
| $\{7.\}$ NO2 + OH = HNO3             | : arr2(1.15E-11_dp, 0.0_dp, temp)    |
| $\{8.\}$ PM10 = PM10                 | : 1.0_dp                             |

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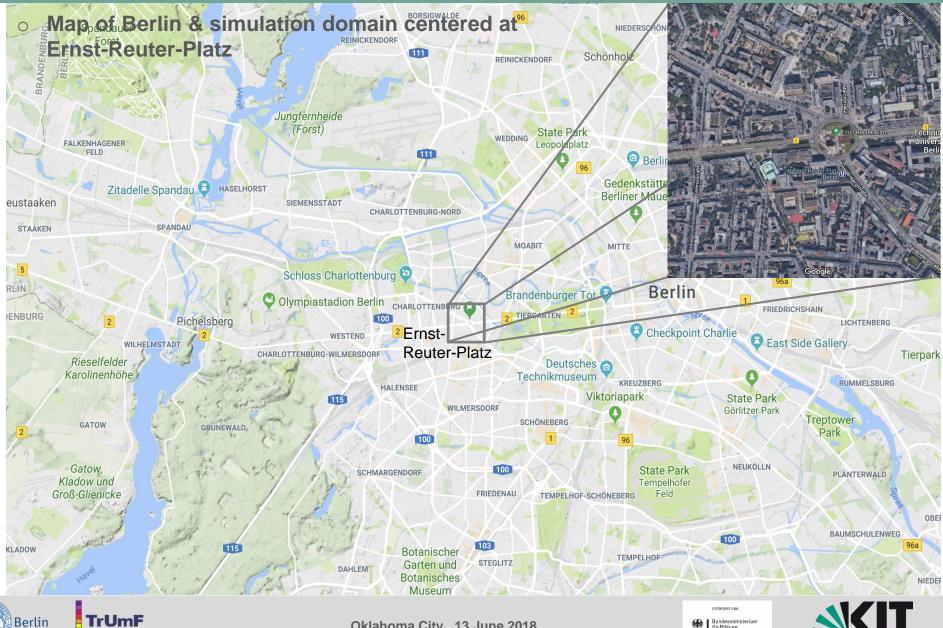
und Forschung



# **Simulation Domain**

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#### [A Case Study-Berlin]





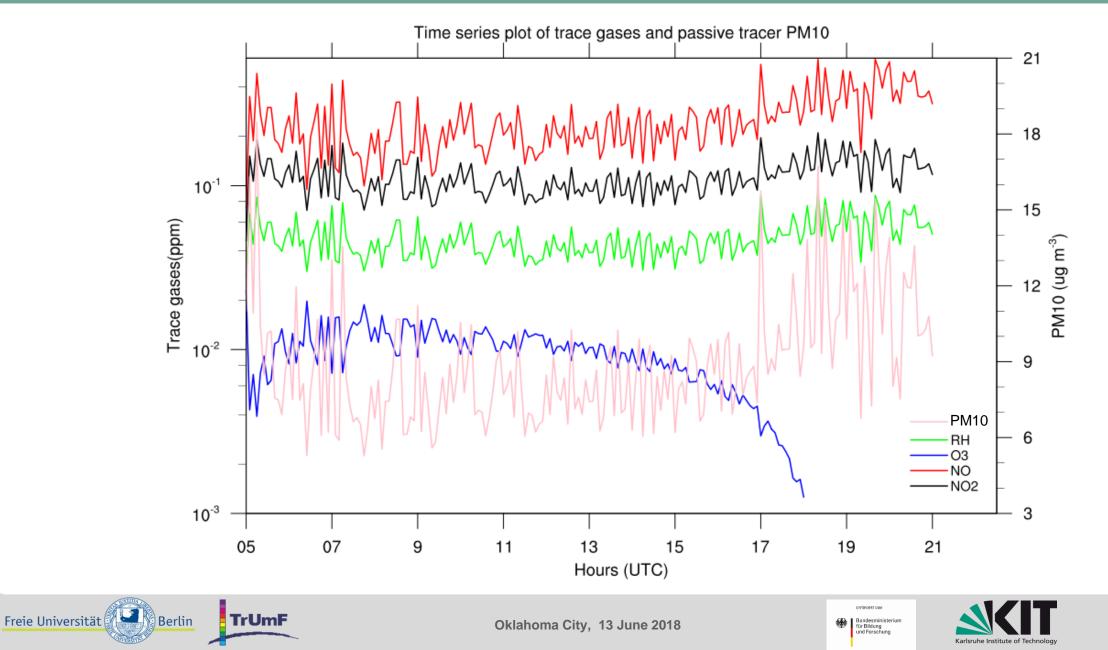
Oklahoma City, 13 June 2018

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#### **Results**

[A Case Study-Berlin]

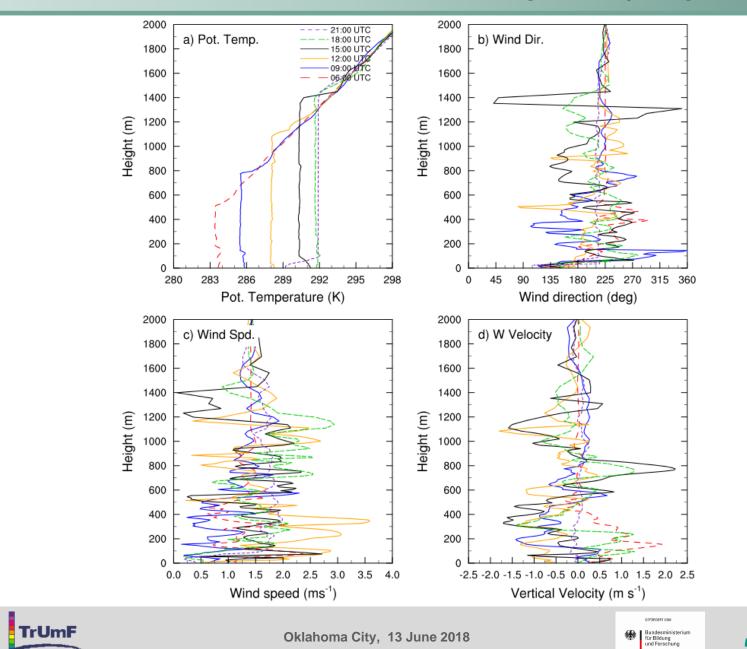




#### **Results**

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[A Case Study-Berlin]



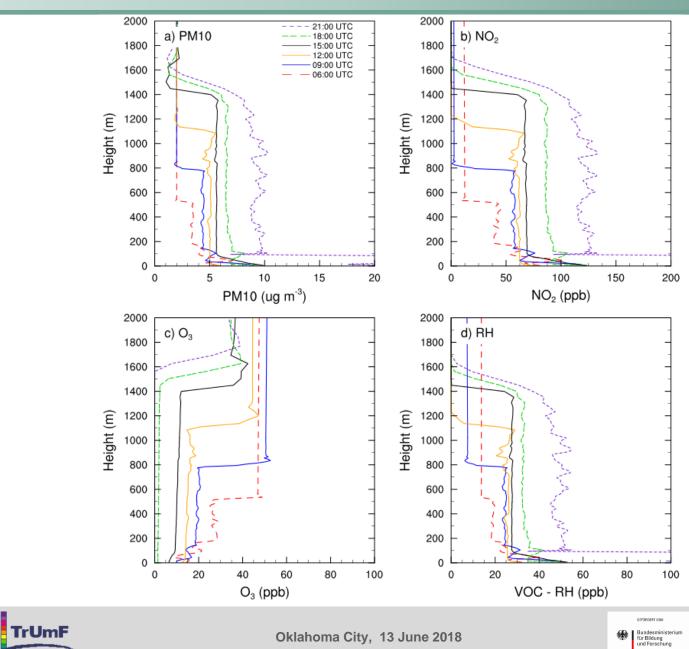




#### **Results**

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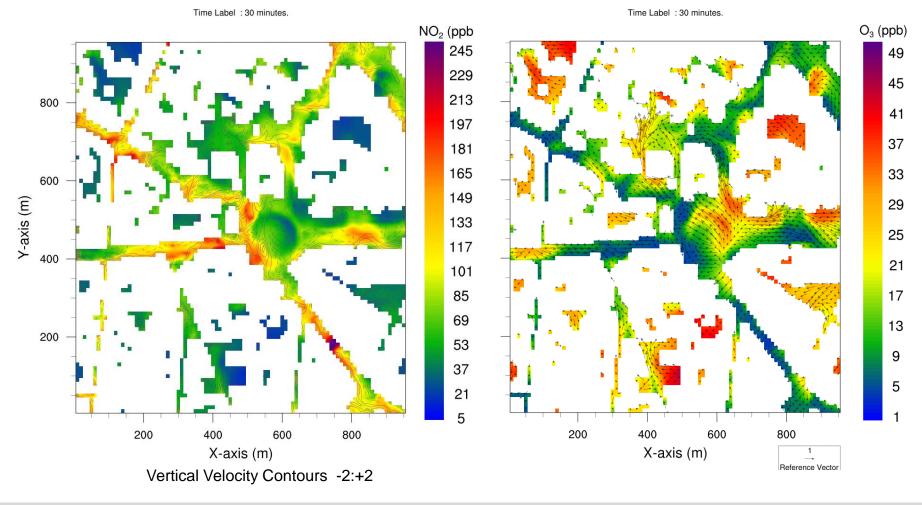
[A Case Study-Berlin]



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Horizontal cross-sections; Level: 5 meter; Left Panel: NO<sub>2</sub> shaded, w-Contours, Right Panel: O<sub>3</sub> shadded and horizontal wind vectors.

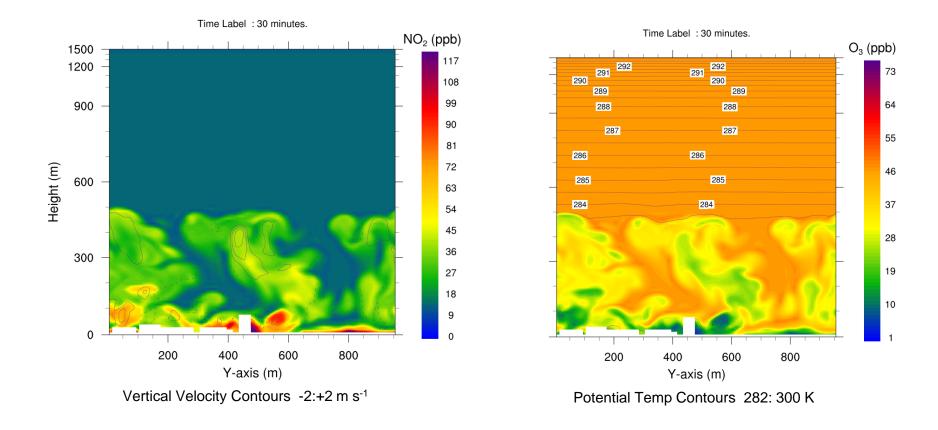


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#### Vertical cross-sections; Left Panel: NO<sub>2</sub> shaded, W-Contours, Right Panel: O<sub>3</sub> shadded, potential temperature contours.









**KIT-Campus Alpin** 

# **Summary and Outlook**

### **Summary**

- Turbulence and building resolving LES PALM-4U model allows accurate simulation of reaction, advection, and removal of atmospheric trace gases and aerosols at appropriate scales.
- PALM-4U has the potential to be the future state-of-the-art comprehensive urban climate modelling system that could be used for the assessment, prediction and investigation of urban climatology, air quality and city planning of large urban areas.

### Coming soon ...

- Chemistry forcing at the lateral boundaries of the parent domain
- Aerosol chemistry (SIA and SOA). SALSA sectional aerosol model (Kokkola et al., 2008) in the process to be incorporated in PALM-4U.
- Deposition module for chemical species and aerosols.
- Detailed anthropogenic emissions (temporal and spatial disaggregation, VOC split etc.).
- Reynolds Averaged Navier-Stokes (RANS) Mode for larger domain, longer simulations and complex mechanisms.









# Wenn du Luft atmest, solltest Du Dich darum kümmern!



