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Innovative Projects

Development of a new urban climate model based on the model PALM – Project overview, planned work, and first achievements

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Abstract

In this article we outline the model development planned within the joint project *Model-based city planning and application in climate change (MOSAIK)*. The MOSAIK project is funded by the German Federal Ministry of Education and Research (BMBF) within the framework *Urban Climate Under Change ([UC]^2)* since 2016. The aim of MOSAIK is to develop a highly-efficient, modern, and high-resolution urban climate model that allows to be applied for building-resolving simulations of large cities such as Berlin (Germany). The new urban climate model will be based on the well-established large-eddy simulation code PALM, which already has numerous features related to this goal, such as an option for prescribing Cartesian obstacles. In this article we will outline those components that will be added or modified in the framework of MOSAIK. Moreover, we will discuss the everlasting issue of acquisition of suitable geographical information as input data and the underlying requirements from the model's perspective.

Keywords: urban climate, microscale model, large-eddy simulation, urban chemistry

1 Motivation

Over the past decades, the number of people in urban environments has continuously increased. In 2016, about 4 billion people (54.5 % of the Earth's human population) lived inside cities and their surroundings (United Nations, 2016). Due to the limited space, the concentration of people and the density of buildings has increased massively, resulting in a replacement of natural conditions, high energy demand, and increased air pollution. The most distinct effects of the urban environment are the well-known urban heat island, modification of the surface roughness, and increased aerosol emissions from traffic, industry and households. In order to ensure a future worth living in, our cities must be adapted to the drawbacks of a changing global environment with much higher temperatures. The interaction between urban areas and the atmosphere has thus received growing attention in urban climate research over the last decades (Oke, 2006; Kuttler et al., 2017). Numerical models are a useful tool to study the multitude of complex interactions and they can also be used to estimate the effectiveness of these complex adaption strategies for climate change scenarios. Today, building-resolving simulations have become commonly used for this purpose and several models have been established in the German scientific community, such as MUKLIMO_3 (Früh et al., 2011), MITRAS (Schlünzen et al., 2003; Salim et al., 2018), ENVI-met (Bruse and Fleer, 1998) and ASMUS (Gross, 2012). However, some of them still use programming standards that are not state-of-the-art, and few are efficiently parallelized (i.e. they show a lack of scalability on clustered computer systems), limit-

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ing their applicability for large domain sizes. Typically, these models run in RANS (Reynolds-Averaged-Navier-Stokes) mode, where turbulence is fully parameterized. Nowadays, however, computer capabilities allow for employing the large-eddy simulation (LES) technique instead, in which the bulk of the turbulence spectrum is explicitly resolved. By resolving these dominant eddies, LES models have the potential to provide more accurate and more reliable results than RANS models (e.g. Letzel et al., 2008; Blocken, 2018). The flow around buildings, for example, can better be described by LES models (see Blocken, 2018, for on overview of advantages and disadvantages of the LES technique). Furthermore, temporal fluctuations can be resolved, which becomes important whenever critical values are involved (e.g. pollutant concentration). On the downside, LES models consume somewhat more computation time than RANS models because the time step is limited by the highest wind speed in the model domain. As LES resolve not only the mean flow, but also turbulent fluctuations, the maximum wind speeds and hence the time step needed can be a factor of two smaller.

In this context, the German Federal Ministry of Education and Research (BMBF) in 2015 announced a call for project proposals with the goal to develop a new and highly efficient urban climate model (UCM). In the framework of the Urban Climate Under Change ([UC]^2) research programme (see offical webpage at http://u2-program.org), UCMs are defined as numerical models that are able to represent the atmospheric processes in the urban canopy layer that are modified by human activity and which constitute the urban microclimate. Despite the fact that the term climate is usually used in connection with 30-year-aggregated data, UCMs are often applied to study atmospheric processes on small temporal (hours to day) and spatial scales (meters to kilometers) instead (see also definition in Scherer et al., 2019a, in this issue).

The call came along with a summary of essential requirements for the new UCM:

- allow for microscale simulations of horizontal domain sizes of up to 1,000–2,000 km^2,
- ability for building-resolving simulation at a grid spacing of $\leq$ 10 m,
- an interface in order to read and use digital surface model data,
- an option for nesting in, or large-scale forcing to, mesoscale numerical forecast models,
- state-of-the-art multivariate data output interfaces, such as NetCDF,
- open source or freeware,
- applicability on desktop computers as well as on massively parallel computer clusters,
- a user friendly interface and interpretation guides that allow even non-experts (e.g. city planners) to conduct simulations,
- and consideration of socio-economic aspects in the model.

Figure 1: The official PALM-4U logo.

Based on this list of requirements, we realized that the Linux-based large-eddy simulation code PALM for atmospheric boundary layer flows (Raasch and Schröter, 2001; Maronga et al., 2015) was an ideal basis for such a new UCM. PALM has been developed at the Institute of Meteorology and Climatology at Leibniz Universität Hannover (LUH) for more than 15 years. PALM is fully parallelized and has shown outstanding scalability on up to several thousands of processor cores (Maronga et al., 2015), being a prerequisite for a modern LES model. PALM follows a state-of-the-art programming standard and is regularly adapted to all kind of new hardware architectures. As it has been increasingly used for urban applications in the past (e.g. Letzel et al., 2008; Inagaki et al., 2011; Park et al., 2012; Abd Razak et al., 2013; Park and Baik, 2013; Yaghoobian et al., 2014; Park et al., 2015; Kondo et al., 2015; Gronemeier et al., 2015; Wang et al., 2017), it is also already equipped with features such as a Cartesian topography model. Furthermore, it has been distributed as open source model under the GNU GPL v3 and uses NetCDF as standard data output format. It is working on both parallel computing clusters with thousands of processor cores but also on powerful workstations with a few tens, and even on desktop computers with only few cores or even only a single core (in a serial mode).

In this context, we designed the project *Model-based city planning and application in climate change (MOSAIK)* (see project web page at http://uc2-mosaik.org) that is funded by BMBF since June 2016 as module A within the [UC]^2 framework. The main goal of MOSAIK is to develop a proper UCM, with PALM as its model core, and by adding all additionally required components to it. The new UCM will be named PALM-4U (*PALM for urban applications*, read: PALM *for you*, official logo shown in Figure 1). In order to guarantee success of MOSAIK and owing to the limited time of funding (three years), we decided to consider only state-of-the-art methods for PALM-4U that are established in the scientific community instead of developing entirely new ones. Also, we decided to exclude the solid and liquid phase of water (that is, precipitation and clouds) within these first years to keep the work programme feasible.

For more details on the [UC]^2 programme and the projects funded see Scherer et al. (2019a) ([UC]^2), Scherer et al. (2019b) (3DO, module B), and Halbig et al. (2019) (KliMoPrax and UseUClim, module C). All papers are published in this issue.

In this article we will outline the work program planned within MOSAIK to develop PALM-4U. Moreover, we will discuss the issue of input data acquisition which plays a key role not only for model operation, but also for the process of model validation. The paper is organized as follows. Section 2 gives a brief summary of the state of the art, an outline of the present capabilities of PALM and the planned PALM-4U enhancements as well as a presentation of the MOSAIK consortium. Section 3 then describes the work programme and Section 4 gives a summary and an outlook on future work.

2 Introduction

2.1 State of the art

Besides field measurements, remote sensing, and wind tunnel experiments, building-resolving numerical models can be used to study atmospheric processes in urban environments. The wide variety of numerical models ranges from general computational fluid dynamics codes to specific meteorological microscale models. An overview is given, e.g., by Toparlar et al. (2015). For urban applications, RANS models have been used in the past to simulate atmospheric conditions for limited areas but also with high numerical resolution. These models have been verified against wind tunnel experiments (e.g. VDI-guidelines 3783, 2017a), but only for mean quantities. On the one hand, for a number of problems in the field of urban microclimate, like the urban heat island effect or thresholds of European air quality standards, mean quantities are significant and the adequate measures. On the other hand, RANS-type models fail whenever fluctuating quantities are adequate and required, e.g., in the field of wind comfort or peak concentrations of air pollutants. Here, turbulence-resolving (i.e. LES) models are necessary to provide realistic solutions.

LES models have been used since more than 40 years for basic research questions. The model setups are often idealized (e.g. homogeneous, flat surface, cyclic horizontal boundary conditions, etc.) and such idealized studies have also been carried out for urban environments, e.g. simple rectangular street canyons (Li et al., 2006) or arrays of regularly-shaped buildings (Castillo et al., 2011). The limitation to idealized setups were a tribute to the large computational resources required by LES. However, the recent and rapid progress in computer hardware meanwhile allows for very realistic urban simulations with both high spatial resolution and large model domains which cover complete city districts or even whole cities. Respective studies have been done by different research groups all over the world and were mainly based on the PALM LES code. Some examples of such urban PALM applications have already been mentioned above. First LES simulations including the transport and dispersion of reactive scalars, e.g., were conducted by Baker et al. (2004), who studied the NO-NO_2-O_3 chemistry and dispersion in an idealized street canyon. Since then, other authors have added more chemical reactants and mechanisms into LES schemes, for example the formation of ammonium nitrate aerosol including dry deposition (Barbaro et al., 2015).

2.2 PALM – the model core

Originally, the name *PALM* was the abbreviation for *the Parallelized Large-eddy simulation Model*, which refers to the parallelization as a special feature of the model. As a matter of fact, PALM was one of the first parallelized LES models for atmospheric flows. The full name was still used recently in this very form in the official model description of version 4.0 (Maronga et al., 2015). However, nowadays all LES models are parallelized, and so this feature can no longer be regarded as being unique. Nevertheless, the name PALM had already established in the scientific community and was thus maintained to date. In the course of MOSAIK, however, we finally decided to drop the full name and use the abbreviation PALM (or PALM-4U in the case of urban simulations) as proper name in the future.

PALM is based on the non-hydrostatic, filtered Navier-Stokes-equations in Boussinesq-approximated or anelastic form. The model solves prognostic equations for the conservation of mass, energy, and moisture in Cartesian space on a staggered Arakawa-C grid. Filtering is achieved by volume-averaging. The subgrid-scale turbulence parameterization follows the 1.5-order scheme after Deardorff (1980) in the formulation of Saiki et al. (2000). Discretization in space is achieved via finite differences and equidistant horizontal grid spacings using a 5th-order advection scheme (Wicker and Skamarock, 2002), while discretization in time is achieved employing a 3rd-order Runge-Kutta scheme (Williamson, 1980). By default, the bottom boundary of the model is flat and a constant flux layer is assumed between the surface and the first atmospheric grid level. Horizontal boundary conditions are by default cyclic. However, PALM also allows non-cyclic boundary conditions using advanced inflow and turbulence-recycling methods (Lund et al., 1998; Kataoka and Mizuno, 2002; Maronga et al., 2015).

PALM also offers a Cartesian topography model, in which topographic elements like complex terrain and buildings are represented as solid obstacles in the code. The topography model currently is designed to resolve

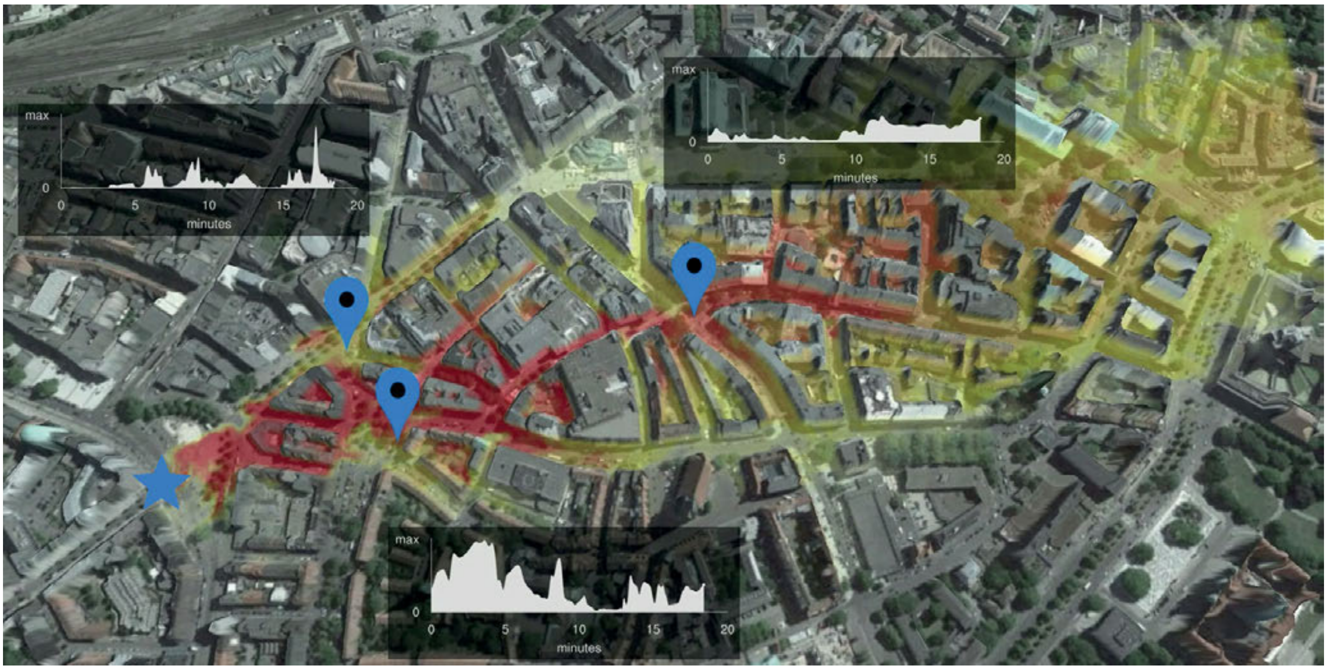

Figure 2: Visualization of the instantaneous concentration of an arbitrary passive pollutant in the Steintor area within the city center of Hannover (Germany). This LES of a neutral boundary layer flow with a geostrophic wind of 8 m s^{-1} was conducted at a grid spacing of 2 m with a prescribed continuous point source at the open space in the lower left part of the figure (indicated by the star symbol). Shown is the pollutant concentration below average rooftop (*yellow* indicate low concentrations and *red* high concentrations). Additionally, time series of the concentrations at pedestrian level at three given locations (marked by the blue spots) are given for a period of 20 min. Satellite images are © DigitalGlobe. VAPOR (Clyne et al., 2007) was used for rendering. The figure was taken from an animation by Gronemeier et al. (2017).

the dynamic effects of the buildings, but it also features an option for prescribing surface fluxes of sensible and latent heat at any of the facade elements. However, the model (version 4.0) lacks fully interactive walls, i.e., an energy balance solver for building surfaces. Figure 2 shows an exemplary snapshot of a PALM simulation of pollutant dispersion in an urban environment with explicitly resolved buildings.

Moreover, a land surface model (LSM) was recently implemented in PALM (for a brief description see Maronga and Bosveld, in press). The LSM consists of a multi-layer soil model, treating the vertical transport of heat and liquid water in the soil, as well as an energy balance solver for the surface temperature. The LSM takes into account the effect of unresolved vegetation canopy, bare soils, as well as interception water from precipitation on plants. In the course of the LSM implementation, a simple clear-sky radiation model was added and the Rapid Radiative Transfer Model (for Global models, RRTMG, Clough et al., 2005) was coupled to PALM as a second option. Large vegetation elements, such as tree stands, can be treated explicitly by a simple canopy model that acts as a sink for momentum using a drag approach over multiple grid volumes.

PALM has shown remarkable scalability that enables the use of large grid domains and small grid spacings. Figure 3, e.g., shows the scaling behavior of PALM for a large-scale test case with 4320^3 grid points with up to 43200 cores, starting with a minimum of 11520 cores. Results for smaller setups and more details are given in Maronga et al. (2015). For a comprehensive overview of PALM 4.0 see Maronga et al. (2015).

2.3 PALM-4U – planned capabilities and application scenarios

As discussed above, MOSAIK aims at adding all those components that are currently missing in PALM and which are relevant for urban applications. In particular, PALM-4U shall be able to predict the atmospheric flow as well as temperature and humidity in urban environments with resolved buildings. This requires an energy balance solver for all facade elements, including calculation of the radiative transfer in the urban canopy layer. This also involves the treatment of heat transfer in solid building walls, through windows, green facades, and roofs. In addition, when going to resolutions in the order of 1 m, trees and shrubs can cover several grid volumes and require adequate treatment. In order to assess anthropogenic effects on the urban atmosphere through air conditioning, an indoor climate model is required that predicts both indoor temperature as well as energy demand of buildings and waste heat. Furthermore, air pollution is a known issue in urban environments and requires the consideration of chemical reactions, emission, deposition, and transport of substances, including reactive species. In order to evaluate the comfort of people in cities, and to take into account socio-economic data

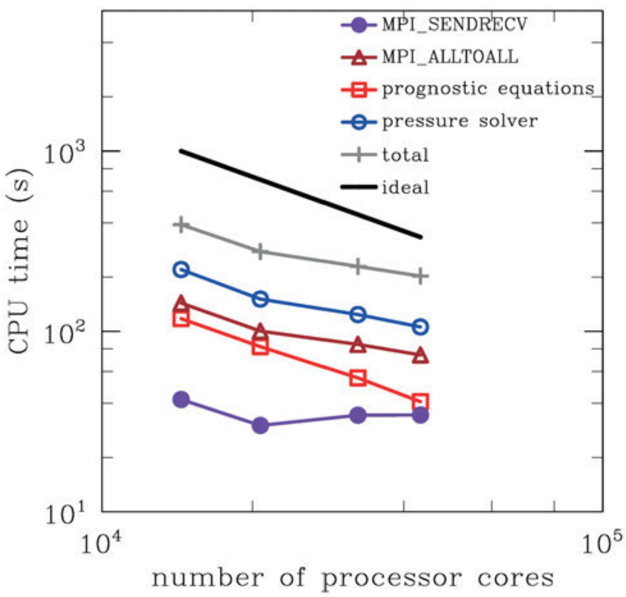

Figure 3: Scalability of PALM 4.0 on the Cray XC30 supercomputer of the North-German Computing Alliance (HLRN). Simulations were performed with a computational grid of $4{,}320^3$ grid points (Intel-Haswell CPUs). Data is shown for up to 43,200 processor cores. Measurement data is shown for the total CPU time (gray line), pressure solver (blue line), prognostic equations (red line), as well as the MPI calls `MPI_ALLTOALL` (brown line) and `MPI_SENDRECV` (purple line). Reprint from Maronga et al. (2015).

in the model, the calculation of key biometeorological parameters is planned. This also involves the implementation of a multi-agent system that will be coupled to the biometeorological estimation.

In order to allow to force PALM-4U with external data from numerical weather prediction models, an advanced interface is needed to feed in respective data to the UCM. Also, state-of-the-art UCMs traditionally use a RANS mode instead of LES mode, which is especially suitable for coarse grid spacings. A RANS mode will thus be essential, and will allow a straightforward coupling to numerical weather prediction models such as COSMO-DE (operational regional model of the German Meteorological Service). Two-way self-nesting of PALM-4U will allow to simulate large areas at relatively coarse resolution, and using a nested domain with much higher resolution, e.g., for single city quarters to obtain high-resolution information in these areas. Building parameterizations for coarse grid resolutions, when buildings are not resolved explicitly, will be needed for simulations of larger domains that include both, entire cities as well as the surrounding (often rural) area, e.g., for studies on the urban heat island effect.

Finally, a graphical user interface with the possibility to prepare input data, initiate PALM-4U simulations, and to visualize results will guarantee user-friendliness and facilitate the application of PALM-4U even for non-expert users.

With these model extensions, PALM-4U will be a comprehensive tool for studying the urban canopy layer with its multitude of different surface types and its feedback on the urban atmosphere. Typical scenarios for the application of PALM-4U are city-wide simulations of the atmospheric flow at typical resolutions of 10 m or less and domain sizes of up to 2000 km^2. The self-nesting approach will allow to use the model as a magnifying-lens tool to look at specific locations of special interest at very high resolution (say domain sizes of 1 km^2 with a grid spacing of 1 m). The simulation period will range from single diurnal cycles to several days, e.g. for high-risk weather episodes like heat waves.

2.4 Participating partners and international cooperations

MOSAIK consists of a consortium of seven research institutes and two small/medium size companies from Germany. The project is coordinated by LUH, which is mostly justified by the fact that LUH is the host of PALM and has gained outstanding knowledge on meteorological model development and model optimization. Also, a majority of the PALM-4U core development is performed at LUH. Table 1 outlines the list of MOSAIK partners and their field of work in context of MOSAIK.

Within MOSAIK, two international cooperations have been established already. First, with A. Hellsten at the Finnish Meteorological Institute (FMI) in Helsinki, who is cooperating closely with LUH to develop an LES-LES nesting for urban simulations and which will speed up the progress with the nesting features planned in MOSAIK. Second, J. Resler and colleagues from the Czech Technical University (CTU) in Prague have developed a preliminary version of an urban surface module (USM) for PALM, based on the existing LSM. The USM consists of an energy balance solver for facades and a heat transfer model for solid walls as well as a radiative transfer model for the urban canopy. A first validation of the USM is published in Resler et al. (2017).

3 Work program

In the following, the work program for the MOSAIK project is outlined and that is planned to be completed within the three years of funding by BMBF.

3.1 Model development

3.1.1 Turbulence parameterizations

Two new turbulence parameterizations will be implemented in PALM-4U. First, a RANS-type turbulence parameterization that will be an alternative option for the currently used subgrid-scale turbulence parameterization. In more detail, a so-called TKE-ϵ-parameterization (Kato and Launder, 1993; Lopez et al., 2005) will

Table 1: List of institutions involved in MOSAIK

Institution	Principal investigators	Function / field of work
Leibniz Universität Hannover (LUH)	Günter Groß	Coordination, energy balance solver, multi-agent system
	Björn Maronga	Coordination, turbulence parameterizations, nesting, benchmarking, energy balance solver
	Siegfried Raasch	Turbulence parameterizations, nesting, benchmarking
	Gunther Seckmeyer	Human biometeorology
Karlsruhe Institute of Technology (KIT)	Renate Forkel	Urban chemistry
	Matthias Mauder	
Humboldt-Universität zu Berlin (HUB)	Sebastian Schubert	Urban radiation, urban parameterization
Offenburg University (HO)	Jens Pfafferott	Indoor climate and energy demand
Freie Universität Berlin (FUB)	Sabine Banzhaf	Urban chemistry
German Aerospace Center (DLR)	Wieke Heldens	Geographical information data
	Julian Zeidler	
GEO-NET GmbH (GEO-NET)	Björn Büter	Data management and user interface
	Dirk Pavlik	
German Meteorological Service (DWD)	Kristina Winderlich	Preprocessing of COSMO-DE data, model testing
	Andreas Matzarakis	Human biometeorology
Ingenieurgesellschaft Prof. Dr. Sieker mbH (IPS)	Heiko Sieker	Soil moisture

be used which is based on two prognostic equations for the turbulence kinetic energy (TKE) and its dissipation rate ϵ. Furthermore, the dynamic mixed-model LES-type parameterization will be implemented which is better suited for coarse grid resolution runs than the currently used Deardorff model.

3.1.2 Parameterizations of non-resolved obstacles

For coarser grid resolutions with grid spacings of > 10 m, suitable parameterizations are needed for all those obstacles that cannot be resolved by the model. We will employ two different approaches to realize this. First, the Double Canyon Effect Parameterization (DCEP, Schubert et al., 2012) in which the urban canopy is represented by street canyons and characterized by the canyons' width, the building height, and their orientation. Second, a more simple approach where building effects will be parameterized as a special "vegetation type" with modified aerodynamic parameters (i.e., displacement height and roughness length adjustment) will be employed.

3.1.3 Nesting and coupling to large-scale models

In order to apply PALM-4U for specific synoptic conditions, like, e.g., heat wave episodes, or even for climate prediction scenarios, it is planned to implement an interface in PALM-4U that allows for using model output of larger-scale models as boundary conditions. An additional software package will be developed that processes data output from COSMO-DE (support for the ICON model chain will be added later) and provides suitable input data for PALM-4U. The processed data will then be used in PALM-4U either as Dirichlet boundary conditions (in RANS mode, default) or as additional tendency terms in the respective prognostic equations (LES mode with cyclic boundary conditions). Moreover, a self-nesting of PALM-4U will be realized, allowing to use the model with a magnifier lens tool. A typical scenario is the simulation of an entire city with explicit buildings at a resolution of about 10 m, with smaller (nested) domains at much higher resolution in the order of 1 m. A first version of such a two-way nesting for the LES mode (LES-LES nesting) using a model coupler has been already realized (see also Section 2.4). Figure 4 shows an example of the LES-LES nesting for an array of cube-shaped buildings. It is very well visible that the domain nested (child domain) within the full model domain (parent domain) displays more small-scale turbulent structures due to the finer grid spacing employed therein. Moreover, it is visible (Figure 4b) that the transition of the resolved structure between the two domains is remarkably smooth. Adaption of the already implemented model coupler for RANS-RANS nesting is straightforward and only requires minor modifications of the LES-LES nesting. Moreover, in order to use COSMO-DE model data with Dirichlet boundary conditions together with the LES mode, it is planned to feed the COSMO-DE data to PALM-4U in the RANS mode, and nest LES domains therein. This will require special treatment of the boundaries as turbulent fluctuations are not provided by the RANS model but are needed as additional boundary conditions in the LES domain. This will be solved using a turbulence generator and so-called buffer zones in the LES domain, where the flow can adjust to the turbulent LES conditions.

3.1.4 Land surface representation

In order to simulate interactions between the atmosphere and the soil-vegetation continuum, an energy balance solver for natural (vegetated and bare soil) and urban (e.g. pavements) surfaces is essential to predict realistic surface conditions and fluxes of sensible heat and latent heat. PALM-4U thus will consist of an energy balance solver for all different types of surfaces as well as an multi-layer soil model to account for vertical diffusion

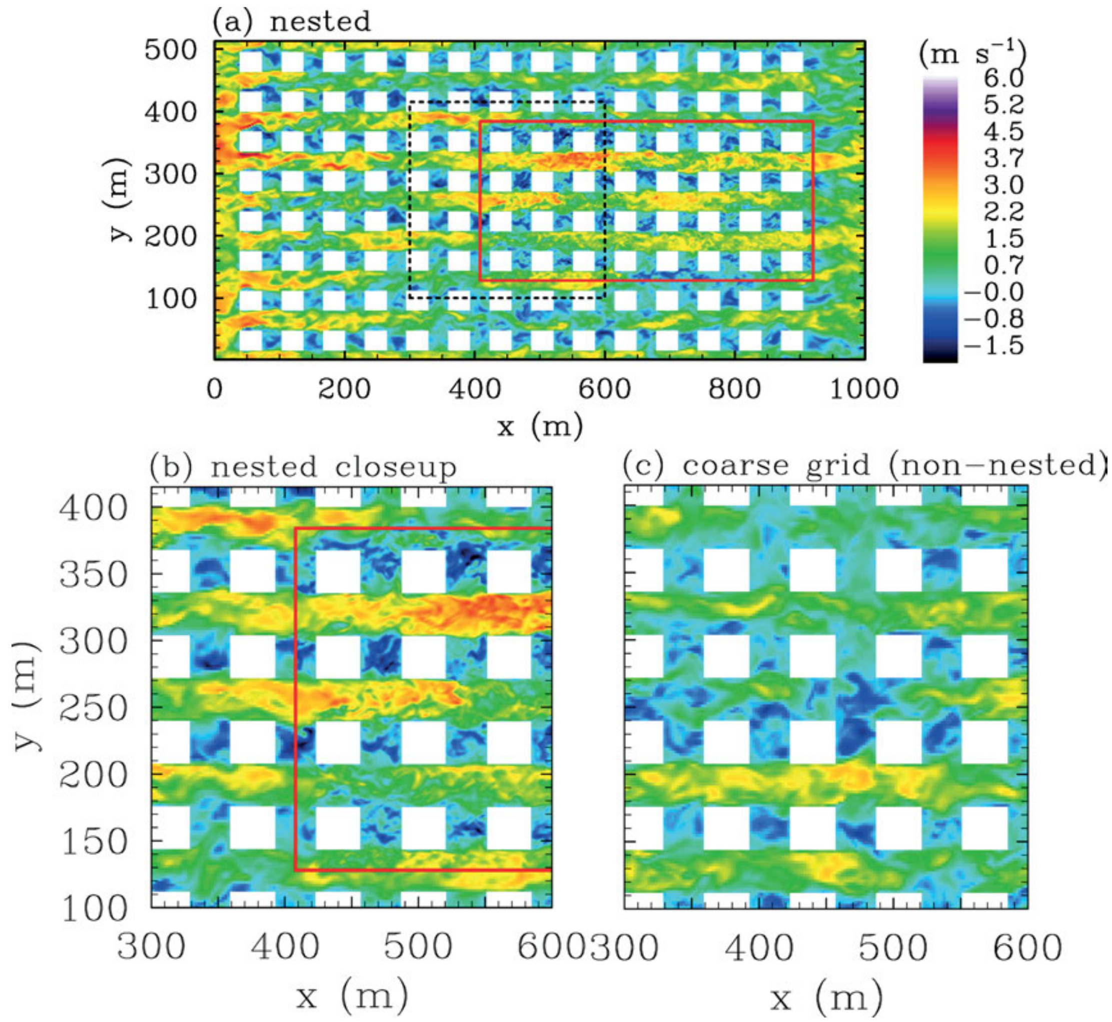

Figure 4: LES-LES nesting applied to a neutral boundary layer flow over an array of cube-shaped buildings. Shown is the longitudinal velocity component (x-direction). A system of two domains with grid spacings of 4 m in the parent and 2 m in the child domain and non-cyclic boundary conditions in x-direction were used. (a) shows the full model domain of the nested system where the child domain is indicated by the red box. (b) shows a close-up view of the area marked by the dashed black box in'(a), while (c) shows the result from a non-nested coarse grid run at 4 m grid spacing for this very close-up region. Please note that the turbulent structure in (b) and (c) cannot be compared as they show instantaneous snapshots where turbulence is localized randomly in the domain. Figure rendered based on data kindly provided by A. Hellsten at FMI.

of heat and water transport in the soil. For natural vegetated surfaces, the energy balance solver will use the concept of a skin layer that has no heat capacity but considers the insulating effect of plants. In the absence of vegetation, no skin layer approach is used and the surface temperature is taken equal to the outermost soil, pavement, or wall layer.

A generalized energy balance equation for the surface (or skin) temperature, T_{surface}, reads

$$C_{\text{surface}} \frac{\partial T_{\text{surface}}}{\partial t} = R_{\text{n}} - H - LE - G \,, \qquad (3.1)$$

where C_{surface} is the heat capacity of the outermost soil or pavement layer, R_{n} is the net radiation at the surface, H and LE are the turbulent surface fluxes of sensible and latent heat, and G is the heat flux into (or out of) the soil. Note that for vegetated surfaces, where the skin layer is applied, $C_{\text{surface}} = 0$. Fluxes are defined positive (negative) when they are directed away (towards) the surface. A full interactive LSM was implemented in PALM, based on the Tiled European Centre for Medium-Range Weather Forecast Scheme for Surface Exchange over Land (e.g. Balsamo et al., 2009) and was first applied by Maronga and Bosveld (in press). Vegetation is fully parameterized, including root extraction of water from particular soil layers used for transpiration and a prognostic equation for the liquid water stored on plants by interception. So far, however, all vegetation is treated to be subgrid-scale, e.g. the canopy has no vertical extent and is parameterized by aerodynamic parameters such as roughness lengths and heat capacity and conductivity of the skin layer.

However, PALM also offers a simple canopy parameterization where plants are explicitly treated using the drag force approach. Therein, vegetation is considered via the leaf area density that can cover several atmospheric grid volumes in 3D space (Maronga et al., 2015; Kanani et al., 2014). In the course of MOSAIK, we will combine both approaches so that it will be possible to resolve the effect of large vegetation (i.e. trees, shrubs) at fine grid spacings by the canopy model, whereas unresolved vegetation (e.g. grass) is treated using the skin layer approach. The canopy model will also be coupled to the soil model so that transpiration from resolved trees is considered by root extraction from the soil. Also, the detailed radiation effect of the resolved vegetation will be taken into account (see Section 3.1.7).

For model initialization, a proper soil moisture content and distribution are often essential prerequisites when permeable surfaces are present in urban areas. Soil moisture, however, reflects the meteorological history of several weeks, including precipitation events, run-off, drainage, and evapotranspiration. In case when specific synoptic conditions are to be simulated, the soil water balance model STORM (Sommer et al., 2008; Sommer et al., 2010) will be used as a preprocessor tool for generating a reliable soil moisture content (and distribution within the soil layers). The required synoptic input data for forcing STORM is provided by COSMO-DE analysis data.

3.1.5 Urban surface representation

In PALM version 4.0, buildings are primarily realized as obstacles that react to the flow dynamics via form drag and friction forces by assuming a constant flux layer between the building surface and the adjacent air volume. A simple thermodynamic coupling is also possible by prescribing surface fluxes of sensible (and latent heat) at any of the building surface grid elements. In order to simulate a realistic urban environment, however, a much more advanced approached will be required. Essentially, this involves the solution of an adapted version of Eq. 3.1 for each urban surface element, such as building facades, roofs and impervious horizontal surfaces like pavement. For solving Eq. 3.1, the radiative transfer in the urban canopy, including multiple reflections and shading from buildings must be calculated, which may be considered to be one of the main challenging tasks in urban surface modeling (see Section 3.1.7). In order to estimate the heat flux G into the material, all building facades must be coupled to a multi-layer wall model. This is further complicated by the fact, that facades can not only consist of solid walls, but usually also consist of significant fractions of windows and sometimes green elements. Windows in particular have significantly different physical properties than solid (greened) wall, e.g. in albedo, and they also allow shortwave radiation to enter the building.

A preliminary version of an urban surface model (USM) has been recently entered the PALM default code (Resler et al., 2017), which already includes an energy balance solver for solid walls (see Figure 5). In the course of MOSAIK we will take this as a basis to add the treatment of windows and green facades using the tile approach. Also, we will couple the USM to an indoor climate and energy demand model (see Section 3.1.6).

3.1.6 Indoor climate and building energy demand

In the current version of the USM, the indoor temperature is assumed to be constant throughout the simulation. When simulating longer periods of time, this is not realistic. In order to calculate the interaction of the buildings with the atmosphere, a holistic indoor climate model (Pfafferott et al., 2011; Pfafferott, 2013) will be added to PALM-4U. This model predicts the indoor temperature and also calculates both the energy demand of each building as well as the waste heat that is released to the atmosphere. The model will be integrated as an optional module that is coupled to the wall model by using the temperature of the innermost wall layer of the respective building facades as input parameter. Also, the transmitted radiation by windows is transferred to the indoor model. The indoor temperature is then calculated based on building characteristics (e.g. insulation, air conditioning, and heating). In return, the indoor temperature is transferred to the wall model as boundary condition, while waste heat from heating or air conditioning is fed back into the atmosphere as an additional tendency in the prognostic equation for temperature at the roof top (representing the typical location of chimneys and air conditioning units).

3.1.7 Radiative transfer in the urban canopy layer

While radiative transfer calculations in an idealized atmosphere for flat surface conditions are known to be a computationally expensive task already, the radiative transfer in the urban canopy layer can be considered to add another level of complexity to this task. In particular, shading effects of buildings and trees as well as multiple reflections between different (building) surfaces require elaborated treatment of the radiative transfer within the urban canopy layer. Nevertheless, accurate predictions of the radiation budget for all surface elements is an essential prerequisite for the reliable prediction of the surface temperatures and thus the turbulent surface fluxes of sensible and latent heat. Moreover, photolysis calculations depend on solar irradiation and thus rely on adequate shortwave radiative fluxes (see Section 3.1.8). Finally, information on orbital parameters of the sun and shading by obstructions is essential for assessing biometeorological parameters (see Section 3.1.10).

The first version of the USM in PALM already tackles most of these enormous requirements. It uses the incoming shortwave radiation that is provided by one of the radiation codes used in PALM (i.e. either the clear-sky model or RRTMG) as boundary condition at the top of the urban canopy layer. Direct and diffuse radiation are treated separately. The USM radiation scheme then adds a description of radiation processes within the urban canopy layer, including multiple reflections between buildings. These processes involve the calculation of the

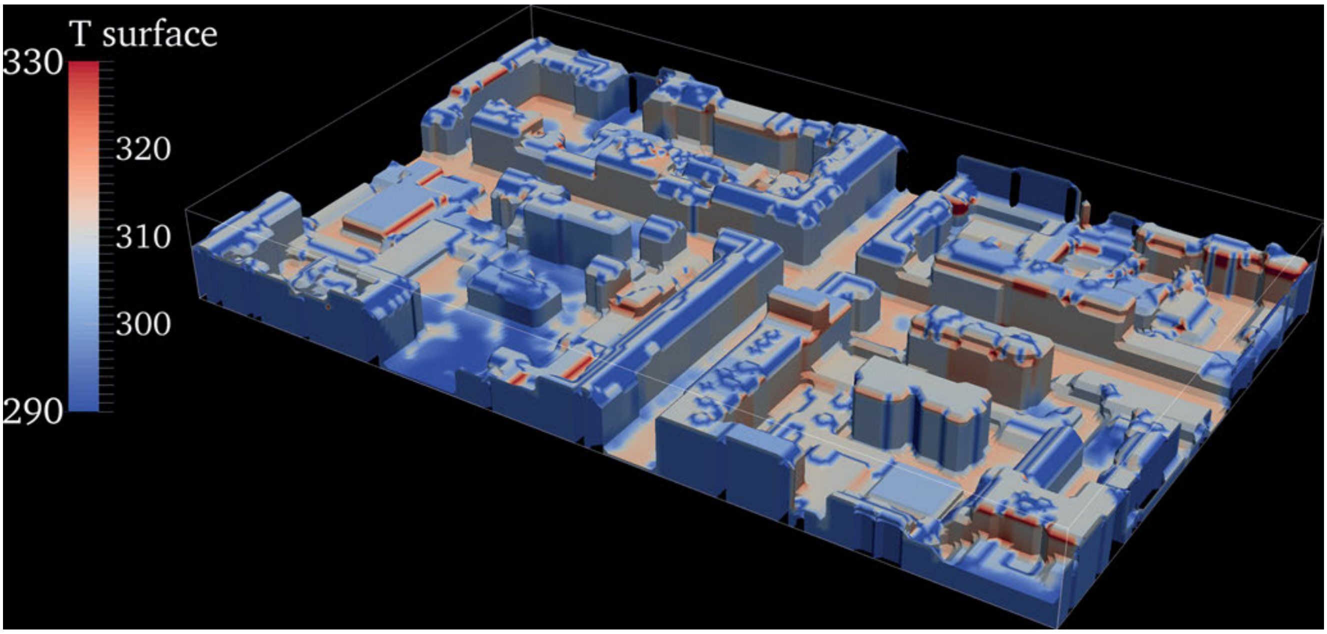

Figure 5: Exemplary 3D visualization of the surface temperature distribution (in K) in the Komunardu city quarter in Prague (Czech Republic) at 3 July 2015, 1300 UTC. The preliminary version of the USM was used to calculate a full diurnal cycle of the surface temperature for a clear sky summer day. The shown horizontal domain size is approximately 400 m × 300 m, where *x*- and *y*-axes are aligned to the west-east and north-south directions, respectively. A grid spacing of 2 m in all spatial directions was used. ParaView (Ayachit, 2015) was employed for rendering. The simulation setup was kindly provided by J. Resler at CTU. A detailed validation of the surface temperatures with field measurements is presented in Resler et al. (2017).

incoming shortwave radiation components on each surface element of the grid, based on the position of the sun and shading according to the geometry of the urban canopy; longwave thermal emission based on the surface temperature of each surface element; finitely iterated reflections of shortwave and longwave radiation by all surfaces; absorption of radiation by individual surface elements based on their properties (albedo, emissivity); and partial absorption of shortwave radiation by vegetation. For details, see also Resler et al. (2017).

Missing radiation processes will be added in the course of MOSAIK. In particular this involves an improved treatment of resolved vegetation for both longwave and shortwave radiation, including the thermal capacity of leaves. Also, as modern architecture often involves glass and polished surfaces, specular reflection might play an important role. Additional work is required to meet special requirements for the urban chemistry to be implemented (e.g. for photolysis, see Section 3.1.8).

In the case of unresolved buildings and vegetation, the radiative transfer will be adapted for the DCEP building parameterization.

3.1.8 Chemistry

Air quality modeling systems consider a variety of physical and chemical processes such as emissions, deposition, transport, chemical transformation, photolysis, radiation and aerosol interactions etc. A fully "online" coupled (Baklanov et al., 2014) chemistry module will be implemented into PALM. The chemical species will be treated as Eulerian concentration fields that may react with each other, and possibly generate new compounds. For the description of gas-phase chemistry the latest version of Kinetic Preprocessor (KPP[1]) version 2.3 has been implemented into PALM-4U (see also Damian et al., 2002; Sandu et al., 2003; Sandu and Sander, 2006). It allows to generate Fortran source code directly from a list of chemical rate equations. A further preprocessor (based on KP4) has been developed that adapts the code to PALM and automatically generates interface routines between the KPP generated modules and PALM. In this way, the chemistry in PALM-4U is fully flexible and easily exchangeable. The PALM chemistry module will be implemented in RANS and LES modes. A more complex chemistry module will be available for the RANS mode, whereas a strongly simplified chemistry mechanism will be available for the LES mode to keep the computational time for chemical transformations and advection of the species at a reasonable level.

The chemistry in LES mode will be based on an equilibrium photo-stationary system and the major pollutants in urban environments. This involves CO and a O_3-NO_2-NO-VOC-HO_x chemistry as well as a small number of products. A preliminary result from a turbulence-resolving (i.e. LES mode) simulation of a small area of Berlin around Ernst-Reuter-Platz, a large roundabout with some high buildings and heavy car traffic is shown in Figure 6. The figure shows surface concentrations of

[1] http://people.cs.vt.edu/~asandu/Software/Kpp/

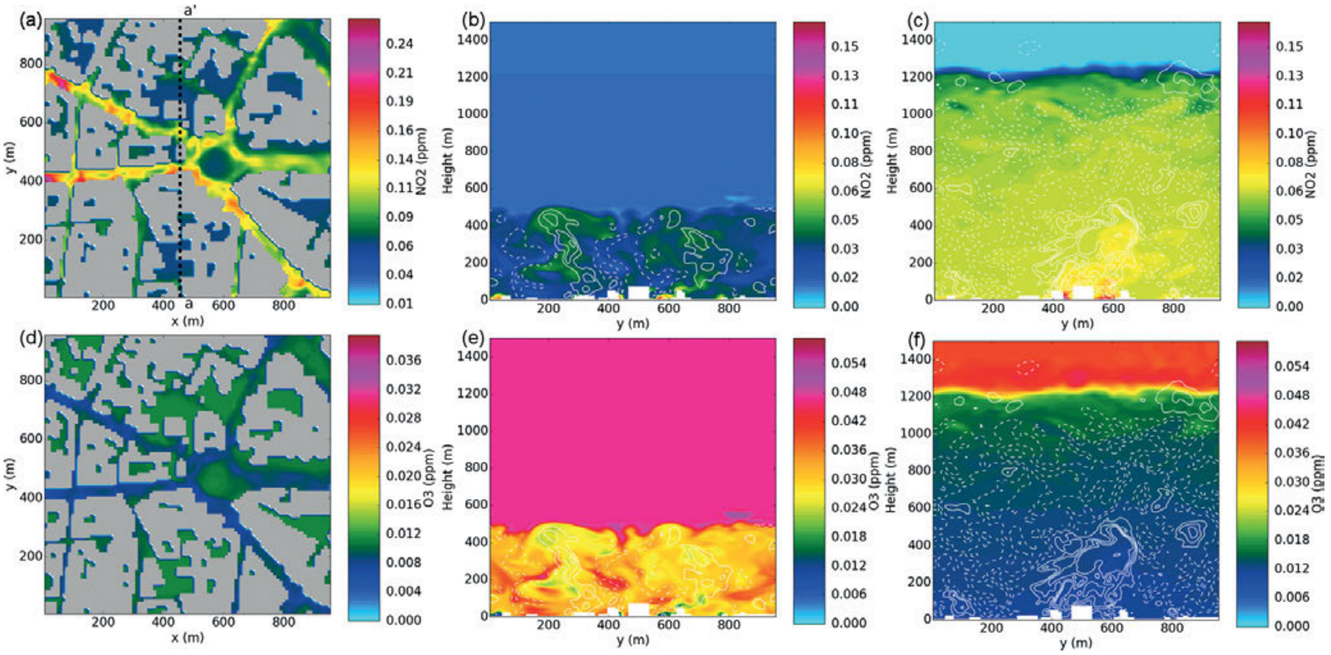

Figure 6: Preliminary results of the chemistry module for an LES of a diurnal cycle for an area around Ernst-Reuter-Platz in Berlin, Germany. Solely traffic emissions were considered which were parameterized depending on the street type classes from OpenStreetMap. Shown are exemplary instantaneous *xy*-cross sections of (a) NO_2 and (d) O_3 at 1330 UTC as well as *yz*-sections (b)–(c) NO_2 and (e)–(f) O_3 during nighttime (0530 UTC, (b) and (e)) and in the afternoon (1330 UTC, (c) and (f)), together with vertical velocity as contour lines. The line a' in (a) indicates the location where the *yz*-sections were taken. The setup for this simulation was kindly provided by B. Khan at KIT.

nitrogen dioxide (NO_2) and ozone (O_3) and matching vertical cross sections at the beginning (nighttime) and a few hours later (afternoon). Figure 6 shows that NO_2 and O_3 vary in space and time due to advection by turbulent motions and chemical transformation of the atmospheric trace gases. Close to the surface NO_2 concentrations are high due to direct emission from traffic and conversion of nitrogen monoxide (NO) to NO_2. The daytime O_3, nitrogen oxides (NO_x, where $NO_x = NO + NO_2$) and VOCs (volatile organic compounds) relation is driven by a complex non-linear photochemistry. Figure 6 depicts a typical VOC-sensitive regime where O_3 concentrations are depressed by NO_x titration. The presented vertical cross sections show that the chemical components are mixed upwards with the gradual increase of the boundary layer from simulation start towards the early afternoon.

In a next step, PM10 and PM2.5 will be implemented as passive tracers. In a third step, a gas-particle phase equilibrium model for the nitrate-ammonium-sulfate system will be included.

In the RANS mode, the chemistry will be consistent with the schemes suggested within current VDI guidelines for regulatory purposes in Germany (VDI-guidelines 3783, 2017b). These will be extended by the particle phase and adapted for their use in the urban canopy. For the secondary anorganic aerosols, different schemes of the SO_4-NO_3-NH_4-H_2O-system will be considered.

Photolysis will be parameterized based on shading information from the urban radiation parameterization and a pollutant deposition scheme will be developed for the deposition to urban surfaces (vegetation, building walls).

3.1.9 Multi-agent system

The conventional approach to assess biometeorological aspects in urban areas is an Eulerian approach, i.e., the area-wide evaluation of relevant parameters and indices (see Section 3.1.10), and subsequent mapping and zoning of these parameters. In this approach, socio-economic aspects of urban residents, such as resident characteristics like age, skin sensitivity, wealth, or population density and the typical behavior and movement patterns of these residents are usually neglected. In order to account for these additional parameters, a multi-agent system will be implemented in PALM-4U that allows a new quality of biometeorological assessment studies. The multi-agent system is a Lagrangian approach in which groups (from hundreds to several thousands) of individual *agents* (i.e., residents) are released at selected locations of interest in the model domain (see e.g. Bruse, 2007; Chen and Ng, 2011; Gross, 2015, for further reading). Each agent can have individual characteristics (age, clothing, speed, starting points, targets, etc.) so that typical population groups can be statistically represented and released in the model. Each agent is able to move according to a path-finding algorithm that takes into account not only the agent's characteristics, but also the atmospheric conditions in its surroundings, like sun/shaded area, searching for an optimal compromise between the fastest and most convenient path. The path-finding algorithm will be based on a potential field scheme where the direction of movement is determined from the sum of forces acting upon the agent. The potential itself can be regarded as the result of a force towards the target area and additional forces due to sloped terrain, forbidden areas (buildings), shaded and non-shaded sites, or the occupation of areas by other agents.

The multi-agent system is suited not only for evaluating biometeorological comfort indices and the relevance of the conventional Eulerian approach, but also for investigating escape routes in case of accidents, possibly associated with release of hazardous and toxic substances.

3.1.10 Human biometeorology

The evaluation of human thermal and wind comfort/stress as well as the exposure to UV radiation will be treated in both the classical Eulerian way, but also in the Lagrangian multi-agent system. Standard biometeorological thermal indices like Physiologically Equivalent Temperature (PET), Perceived Temperature (PT), and Universal Thermal Climate Index (UTCI) as well as wind comfort will be calculated area-wide directly by the biometeorology module in PALM-4U and provided as output data. The module will be based on the existing models RayMan (Matzarakis et al., 2010) and SkyHelios (Matzarakis and Matuschek, 2011). Moreover, a Lagrangian version will be implemented in that sense that the thermal and wind comfort are estimated for the agents released in the urban environment. However, as the established biometeorological indices are only defined for stationary meteorological state, adaptation and possibly re-definition of these indices will be required as the moving agents no longer experience stationary atmospheric conditions.

The actinic module will primarily deal with the UV exposure of agents as they are moving through the model domain. This will be realized by calculating the biologically weighted UV exposure after Seckmeyer et al. (2013), taking into account not only the complex human geometry, but also including various clothing conditions (which are assigned as attributes to the individual agents) as well as the shading of buildings. While this method provides the cumulated exposure of selected individuals, a more general approach will also be used to derive area-wide maps (Eulerian approach), for which exposure rates will be calculated based on idealized typical human geometry and clothing.

The biometeorological module will not only allow to automatically obtain relevant parameters for stress/comfort. The calculated indices and parameters will also be able to be incorporated into the path-finding algorithm of the multi-agent system. For example, excessive UV exposure in summer time might lead to a lower resistance for those surface areas that are shaded by buildings and vegetation and which thus are favorable. In this way, the agents can adjust their way through the urban area with improved comfort.

3.2 Graphical user interface

Complex meteorological models such as PALM (and thus PALM-4U) usually require fundamental knowledge of both the physical framework implemented in the model, and the technical-numerical implementation. Extensive experience is an essential prerequisite for the successful application of such models. PALM-4U, however, shall be suitable not only for scientists that have a strong background in boundary-layer meteorology, but also for staff of climate service companies; and even for administrative staff with a suitable training. In order to achieve this, both the model setup generation as well as the model steering require substantial simplification. Also, data handling and storage as well as visualization of model output obviously are important tasks in this context. Therefore, a user-friendly graphical user interface will be developed. The web-based interface will allow to generate suitable input data and will make use of tools to convert and modify GIS data which are available in a central database or which are provided by the user. The user will be able to select the forcing of the model, e.g. by a meteorological setting, or by scenario data. A selection of typical synoptic conditions (e.g. heat waves) will be delivered along with PALM-4U. Also, the interface will allow to select and gather data from the COSMO-DE model to simulate realistic synoptic conditions. As PALM-4U's model physics and numerics are very complex, creating a valid model setup that produces reliable results can become a challenging task that can only be achieved by expert users, the graphical user interface will focus on a limited number of typical use cases for which ready-to-use setup files will be provided. The specifics of these use cases will be defined in consultation with the partners from module C (Halbig et al., 2019).

3.3 Geographical information input data

A major task for urban modeling is the acquisition of suitable geo-spatial information data and its incorporation in the modeling system, starting with information on building heights and terrain, and more complex information like vegetation, soil texture, etc. When going to grid spacings down to 1 m as envisaged with PALM-4U, spatial information on all surface elements is required at pixel size (i.e., at a scale of 1 m^2), including characteristics of walls, windows, and green roofs/facades. Moreover, soil properties and information on all different kind of vegetation within the urban environment are needed to accurately predict the urban meteorological conditions for a specific setting. Such information is almost impossible to obtain at the meter-scale. Wherever suitable data is not available (which is rather the common situation than the exception), reasonable assumptions must thus be made and the input data must be simplified. For example, exact building wall textures (color, window fraction, wall material, insulation) are usually difficult to obtain. By the same token, the output data and hence the model quality highly depends on the adequate representation of all these input parameters so that a proper evaluation and validation of the model itself is a challenging task.

In order to facilitate a proper evaluation of PALM-4U, we will make an effort to collect and process an extensive data set of input parameters for the so-called demo-cities Berlin, Stuttgart, and Hamburg (Scherer et al., 2019a, 2019b). As most of the required data is not (freely) available, they must be derived from suitable data sources, above all from satellite data (this will be covered by the MOSAIK partner DLR, see Table 1). Further sources involve available data from the local municipalities, e.g. land use, soil type, and vegetation. Here, we are facing the eminent problem that there is *de facto* no existing data standard in Germany on what data is available for a specific city and in which format and level of detail this data is stored. Also, the availability is not regulated so far. This constitutes a general problem for urban climate modeling, as the model itself is confronted with the non-existence of data standards and thus various data formats. In the conception phase of MOSAIK and $[UC]^2$ a standard interface was defined that is based on the NetCDF data format (called PALM-4U Input Data Standard, PIDS). The PIDS describes in detail how geo-spatial data must be provided as input for PALM-4U. Preprocessing tools will be developed for the most common geo-spatial data formats (e.g. shape files) to convert arbitrary data to the PIDS.

3.4 Model validation

All new components of PALM-4U will undergo strict technical testing. This involves a) code verification, b) Benchmarking, and c) internal validation. Code verification involves checks for compliance with the PALM-4U Fortran coding standard, testing for run-time errors, and compiler-dependent code functionality. If the individual components pass these first tests, benchmark runs will be conducted to assess the scalability of these components on both small (e.g. 4) and large number (e.g. 4,000) of processor cores in order to ensure the applicability of the model for large-scale simulations, for instance for large cities. The internal validation basically involves first comparisons of the model with results from existing UCMs like ENVI-met to check for plausibility of results. Moreover, existing wind-tunnel data for well-described setups will be used for a first validation of the model.

Systematic and thorough model validation, however, will be joint activity of the MOSAIK consortium and the partners from 3DO. It is planned that all simulations required for validation are performed by MOSAIK, while 3DO will be responsible of conducting the evaluation/validation. For this purpose, wind tunnel experiments will be conducted in the Environmental Wind Tunnel Laboratory at the University of Hamburg. Moreover, intensive observations have been and will be conducted in the selected German cities of Berlin, Hamburg, and Stuttgart. Due to the immense amount of work involved in this process, the evaluation process will be an activity that will outlast the first $[UC]^2$ funding phase and be a key action in the ensuing period. For more details on the validation campaigns and wind tunnel experiments, see (Scherer et al., 2019b, this issue).

3.5 Timeline

Table 2 gives an outline of the PALM-4U development. The beta version PALM-4U that already includes many of the outlined new components was released on December 15, 2017 and is available from http://www.palm4u.org. The first release candiate was rolled out in October 2018 (delay of one month with respect to the planned delivery date).

4 Summary and outlook

In this project description paper we outlined the key objectives of MOSAIK, which is an on-going research project within the framework $[UC]^2$ and funded by the BMBF since 2016. The ultimate goal of MOSAIK is to develop a new and innovative open source UCM that can be applied not only for basic research, but also for applied research and assessment studies. In order to achieve this goal, the highly optimized LES model PALM was chosen as model core for the new UCM. The model already has many required features available, particularly, it offers a Cartesian topography model in order to represent buildings. It is available as open source software and shows remarkable performance. Missing capabilities will be added to PALM in MOSAIK in order to allow the adequate representation of all relevant urban processes like radiative transfer in the urban canopy layer, a solver for the energy balance of urban surfaces, chemistry of different complexity, and an indoor climate model. Besides, a RANS-type turbulence parameterization will be added to allow a straightforward coupling to COSMO-DE and for simulations with coarse grid spacings, where the LES approach is not performing well. Moreover, a multiple nesting mechanism will be realized so that the new UCM can be forced by mesoscale weather forecasting models (e.g. COSMO-DE). Moreover, self-nesting is already under way so that larger domains can be simulated at coarser resolution, while special areas of interest can be resolved with a finer grid spacing. The new UCM will be called PALM-4U and will be distributed, just as PALM, as open source software under GNU GPL v3. In order to make the use of the model possible even for administrative staff with limited knowledge about computational fluid dynamics, a graphical user interface will be developed that takes care of the model steering, preprocessing of GIS data for model input, the meteorological setup, and visualization and analysis of output data.

Given the limited time of the $[UC]^2$ program (three years) and the available resources, we decided to exclude some, yet important, physical processes in this

Table 2: Time line for the MOSAIK project

	2016			2017				2018				2019	
	Apr–Jun	Jul–Sep	Oct–Dec	Jan–Mar	Apr–Jun	Jul–Sep	Oct–Dec	Jan–Mar	Apr–Jun	Jul–Sep	Oct–Dec	Jan–Mar	Apr–Jun
Milestone	M1						M2			M3			M4

M1: Start of the MOSAIK project (June 1, 2016)
M2: Release of PALM-4U beta version (December 15, 2017)
M3: Release of PALM-4U release candidate (September 30, 2018)
M4: Release of PALM-4U (May 31, 2019)

Table 3: List of abbreviations

Abbreviation	Description
BMBF	German Federal Ministry of Education and Research
DCEP	Double Canyon Effect Parameterization
HLRN	North-German Computing Alliance
KPP	Kinetic Preprocessor
LES	Large-eddy simulation
LSM	Land surface model
MOSAIK	Model-based city planning and application in climate change
PALM-4U	PALM for urban applications
PET	Physiologically Equivalent Temperature
PT	Perceived Temperature
RANS	Reynolds-averaged Navier Stokes
RRTMG	Rapid Radiative Transfer Model for Global Models
TKE	Turbulence kinetic energy
UCM	Urban climate model
USM	Urban surface model
UTCI	Universal Thermal Climate Index
VOC	Volatile organic compound
$[UC]^2$	Urban Climate Under Change

first phase of model development. In particular, these are all processes that are related to the liquid and solid phase of water in air, soil, and on the surface. Precipitation might be generally used as input parameter to store liquid water on plants and in the soil, but PALM-4U's capabilities to predict precipitation will be limited to warm clouds at the moment. Also, the incorporation of radiative effects of clouds in the radiation calculation for the urban canopy layer is a difficult task. Further topics related to liquid water in urban environments are surface run-off, drainage, and a more detailed representation of water bodies in urban environments. Furthermore, snow pack is known to have a strong effect on the energy balance of the Earth's surface and thus should be incorporated. Our goal is to tackle these topics in a follow-up project, possibly within a second funding phase of $[UC]^2$.

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