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uDALES: large-eddy-simulation software for urban flow, dispersion, and microclimate modelling

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Summary

With continuing urbanization, challenges associated with the urban environment such as air quality, heat islands, pedestrian thermal comfort, and wind loads on tall buildings, are increasingly relevant. Our ability to realistically capture processes such as the transport of heat, moisture, momentum and pollutants, and those of radiative transfer in urban environments is key to understanding and facing these challenges (Oke et al., 2017). The turbulent nature of the urban flow field and the inherent heterogeneity and wide range of scales associated with the urban environment result in a complex modelling problem. Large-eddy simulation (LES) is an approach to turbulence modelling used in computational fluid dynamics to simulate turbulent flows over a wide range of spatial and temporal scales. LES is one of the most promising tools to model the interactions typical of urban areas due to its ability to resolve the urban flow field at resolutions of $O(1\text{ m}, 0.1\text{ s})$, over spatial domains of $O(100\text{ m})$, and time periods of $O(10\text{ h})$. Although there are many scalable LES models for atmospheric flows, to our knowledge, only few are capable of explicitly representing buildings and of modelling the full range of urban processes (e.g. PALM-4U Resler et al. (2017); Maronga et al. (2020); or OpenFoam Weller et al. (1998)).

uDALES (urban Dutch Atmospheric LES) is an extension of DALES (Dutch Atmospheric LES; Heus et al. (2010), Tomas et al. (2015)). It has the additional functionality of modelling buildings within the fluid domain and therefore the capability to model urban environments at the microclimate scale with wet thermodynamics (Table 1). The uDALES framework includes tools to enable users to model a wide variety of idealized and complex urban morphologies (Sützl, 2021; Sützl et al., 2021). uDALES uses an Arakawa C-grid and typically uses second-order central-differencing schemes. For scalar quantities, e.g. for pollution concentration, it is possible to use a kappa-scheme for advection to ensure positivity (Hundsdorfer et al., 1995). A third-order Runge-Kutta time integration scheme is applied. The immersed boundary method, first introduced into DALES by Pourquie et al. (2009) and Tomas et al. (2015), is used to represent buildings (supporting grid-conforming cuboid geometries; Pourquie et al. (2009)). Wall functions have been added to calculate the surface scalar and momentum fluxes at the rough immersed boundaries (Cai, 2012, 2011; Suter, 2018; Uno et al., 1995), based on a local Richardson number. Additional factors are considered to obtain the evapotranspiration fluxes from vegetated surfaces. The code uses fast Fourier transforms to efficiently solve the Poisson equation for pressure and is fully parallelized using MPI (domain decomposition is performed in the spanwise direction, thus producing slabs).

A novel surface energy balance model has been implemented in a two-way-coupled manner (Suter, 2018) and includes the effect of turbulent exchange of heat between the surface and the air, as well as radiation and thermal conduction within the surface. uDALES has tools

for modelling shortwave and longwave radiative fluxes following a radiosity approach (similar to Aoyagi & Takahashi (2011); Resler et al. (2017)), including calculation of direct solar radiation and view factors (Rammohan Rao & Sastri, 1996), considering shading and multiple reflections.

uDALES also has the tools necessary to study air quality within cities. Both idealized (point and line) and realistic (street network) sources can be implemented and both passive and reactive scalars can be modelled. The code supports null cycle chemistry (NO-NO_2-O_3 reactions), and can be easily extended to more sophisticated schemes (Grylls et al., 2019; Grylls, 2020). The high spatial and temporal resolution enables analysis of e.g. real-time pedestrian pollution exposure.

The modelling capabilities of uDALES outlined above, combined with the ability to devise numerous simulation set-ups (e.g. via different lateral boundary conditions: periodic, inflow-outflow and driver) facilitate a plethora of possible studies into the urban environment. Relevant recent publications and their research applications are summarized in Table 1.

Table 1: uDALES research applications.

Research application	Reference
Urban boundary layers/ boundary-layer meteorology	Grylls et al. (2019); Sützl et al. (2021); Sützl (2021)
Urban climate (radiation, green roofs and walls, trees etc.)	Suter (2018); Suter et al. (2021); Grylls & van Reeuwijk (2021)
Pollution dispersion/ urban air quality	Grylls et al. (2019); Grylls (2020)
Buoyancy/ convective and stable conditions	Suter (2018); Grylls et al. (2020); Grylls (2020); Grylls & van Reeuwijk (2021)

Here we present uDALES, a free and open-source large-eddy-simulation software for urban flow, dispersion, and microclimate modelling. In the current platform on GitHub we include: (i) cross-platform support for GNU, Intel, and Cray compilers on Windows and macOS systems, (ii) continuous integration with build and regression tests to check for compilation and simulation errors respectively (Riechert & Meyer, 2019), and (iii) several pre- and post-processing scripts in MATLAB as well as Singularity (Kurtzer et al., 2017) scripts to address issues of scientific reproducibility (e.g. Meyer et al. (2020)). Current developments include the role of urban trees (Grylls & van Reeuwijk, 2021) and future releases may include the use of PsychroLib (Meyer & Thevenard, 2019) to improve the calculation of psychrometric properties of air, and the ability to simulate the diurnal cycle of the urban microclimate in response to solar radiation (Suter, 2018). A detailed description of the model, including a validation study and an example of the surface energy balance is provided in Suter et al. (2021).

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