

Response to Referee #3:

General Overview: The manuscript titled "A conservative immersed boundary method for the multi-physics urban large-eddy simulation model uDALES v2.0" presents advancements in the uDALES framework, particularly focusing on the implementation of a conservative immersed boundary method (IBM) for urban surface representation. This method aims to address the challenges associated with complex urban geometries in microscale urban air flow simulations. While the paper demonstrates improvements over the previous version of uDALES and provides insights into the capabilities of the new method, several key issues need to be addressed before the manuscript can be considered for publication.

Response: We thank the reviewer for this thorough review. Below, we present a point-by-point response to the issues. Given that addressing the major issues in the manuscript required a fairly large number of changes in multiple locations, for clarity we generally do not include the exact changes made here. Instead, we describe where and how the manuscript has been revised.

Major Issues:

Radiation Interaction and Reflections: One major issue concerns the clarity of the radiation interaction process and reflections in the manuscript. The explanation of how the new method of surface representation improves reflections is not adequately presented. While the authors briefly mention view factors, further details are needed to understand the specific improvements achieved with the new method. Additionally, the validation simulations do not adequately reflect the impact of the improved surface representation on radiation interactions. I believe further clarification and demonstration is needed.

Response: We did not go into detail in this paper since the handling of reflected radiation is conceptually unchanged from uDALES v1. One difference is that the view factor calculation is done using the open-source code View3D, which is capable of handling complex triangular meshes. This however does not change the reflection calculations. The algorithm used to account for reflections is an iterative method that continues until all radiation up to a specified threshold is either absorbed or is reflected to the sky (Suter et al., 2022).

Note that we do not claim that the new geometry representation improves reflections per se; the radiation calculation will be more accurate (for non-grid-aligned geometries) because the walls are no longer limited to being either parallel or perpendicular. The reason the reflections are important is shown in Sect. 4.4 - if the geometry is approximated as being aligned to the grid by using lots of small facets, there can be reflections between facets on the same wall that clearly would not occur otherwise. Such problems would only be compounded if using a geometry with reflections between different walls, for example a street canyon (such a case was in fact considered for Sect. 4.4). Since the reflection algorithm has not changed, we feel that the case presented in the paper validates the new geometry specification sufficiently. To address the reviewer's concerns, we have expanded Sect. 3.4 and emphasised what has changed from v1 and v2, and how exactly this impacts performance and accuracy.

Simplicity of Test Cases: Another major concern is the simplicity of the test cases used for validation, which may not fully capture the complexity of urban environments. The validation simulations should consider a wider range of scenarios to assess the robustness and applicability of the new method in diverse urban settings. Incorporating more realistic urban configurations and environmental conditions would strengthen the validity and relevance of the findings. Otherwise, justification is missing here.

Response: We acknowledge that the cases presented do not capture the full complexity of urban environments. The intention in this paper is to describe and validate parts of the model that have been changed from v1 to v2, and explain the differences

in the results, and the test cases are therefore simple by design. In particular, the paper introduces (to the authors' knowledge) a novel approach for urban LES on Cartesian grids - namely the use of an IBM capable of handling non-grid-aligned surfaces that includes heat transfer. The priority is therefore to demonstrate the validity of this approach at a fundamental level, as
40 bottom-up validation is standard practice when making changes of this magnitude. Using more complex cases (that are not focused on isolating a particular aspect of the model) would make explaining the differences more challenging, and potentially even mask conceptual and implementation errors.

Having made the argument that simple cases are appropriate given the aims of this paper, we acknowledge the need for urban models, including ours, to be validated and compared to each other for realistic urban settings. We have had preliminary
45 discussions to perform an inter-comparison exercise with different urban codes developed by other groups, but this is well beyond the scope of the current paper.

Representation of Resolved Vegetation: The manuscript lacks sufficient detail regarding the representation of resolved vegetation in the simulations. Given the importance of vegetation in urban microclimate simulations, particularly in influencing surface energy balances and pollutant dispersion, it is essential to provide a comprehensive description of how vegetation is
50 incorporated into the model and validated in the simulations. Including relevant references and discussing the implications of vegetation representation would enhance the completeness of the manuscript.

Response: A complete description of how resolved vegetation (trees) are modelled in uDALES is available in Grylls and van Reeuwijk (2021); Suter et al. (2022). This is not an aspect of the model that has changed from v1 and v2, so we prefer not to repeat this description in detail or to re-validate this part of the model. We have further emphasised this in Sect. 3.3.

55 **Increased Computational Requirement:** The introduction of the new triangular surface representation may significantly increase the number of surfaces compared to traditional rectangular surfaces. The potential impact of this increase on the performance and computational requirements of the model should be clarified. Authors are encouraged to discuss any potential implications for computational efficiency and scalability.

Response: Note that the computational performance of the IBM scales linearly with the total number of facet *sections*, rather than the number of facets, and the number of sections depends on total surface area and the grid resolution - we have added
60 this point to Sect. 3.3.2. However, the shortwave radiation-related routines do scale with the number of facets (N), specifically the view factor calculation is $\mathcal{O}(N^2)$, and direct solar radiation calculation was approximately $\mathcal{O}(N^2)$ in uDALES v1 and is now $\mathcal{O}(N)$ in v2. Note that the calculation of net shortwave radiation is a pre-processing step, and so does not affect the performance of the code in the sense discussed in Sect. 3.1.

65 With respect to triangles vs quadrilaterals, indeed converting a given quad mesh to a tri mesh by repeatedly dividing each quad by 2 will result in at least twice as many faces – see Sect. 4.1, and also 4.3/4.4 where uDALES v2 uses more facets than v1 in the non-rotated case. However, it is not necessary to generate the mesh in this way - see Sect. 4.2, where it is not clear that fewer quads than tris can be used to represent the building. Also, the fact that the radiation routines scale better and practically run faster means that v2 will tend to perform better even if N is larger. We have added a discussion of these points to Sects.
70 3.3 and 3.4.

Accuracy of Numerical Solution: The scheme now resembles somewhat an unstructured grid, which may raise concerns about the accuracy of the numerical solution due to increased numerical errors. Authors should address whether this change

affects the accuracy of the solution and discuss any measures taken to mitigate potential errors (if any). The discussion should compare the accuracy with the traditional unstructured grid given here: <https://doi.org/10.1016/j.buildenv.2008.11.010>.

- 75 **Response:** While the geometry representation is unstructured, uDALES v2 still uses a Cartesian computational grid, with an immersed boundary method to model the geometry. The governing equations and discretisation of the LES are unchanged from v1, therefore the accuracy is too. The key difference is how the surface fluxes are calculated (using the wall functions). For non-grid-aligned surfaces, there are some considerations to do with grid resolution (relating to the distance to the wall) that were not included in the original text and have been added in Sect. 3.3.2 and Appendix B. This issue aside, the wall functions
- 80 should not be affected much by spatial discretisation (at least not more so in v2 than v1) as they are physical parametrisations. We have added a mention of the use of unstructured meshes, using the provided reference, in the Introduction.

Minor Issues:

- Introduction Citations:** The introduction section lacks citations to support the background information provided. For example, lines 28-29 and lines 35-36 may benefit from adding some references, such as <https://doi.org/10.1016/j.enbuild.2023.113324>,
- 85 which exemplify the application of micorscale urban climate models in realistic urban environments. Also the radiation model of PALM in line 54 (<https://doi.org/10.5194/gmd-14-3095-2021> and <https://doi.org/10.5194/gmd-15-145-2022>)

Response: We have added the references to PALM in the Introduction, and added the other reference to the Conclusion as an example of the kind of studies that are now possible with uDALES v2.0.

- Additional Models in Introduction:** Lines 37-39 should include references to other relevant models such as MITRAS, MISKAM, etc., to provide a comprehensive overview of existing approaches in the field.
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Response: We have added a reference to MITRAS (Salim et al., 2018) in the Introduction.

Temperature Scale in Figure Legend: The temperature scale in the legend of figure 1 has a minimum and maximum of 300K. Additionally, the caption of the figure should be more informative to provide clear context and interpretation of the results.

- Response:** The temperature field is not in fact relevant. We therefore have opted to replace Fig. 1 (see below), which shows
- 95 the problem with representing realistic geometries in uDALES v1 with respect to radiation.

Relevance of Certain Text: Lines 74 - 77 may not be necessary and could be considered for removal if they do not contribute to the manuscript.

Response: We would prefer to keep these lines, as some readers might find this useful.

Organization of Content: Line 153 should be moved to the relevant subsection for better organization and clarity.

- 100 **Response:** We have moved this sentence to the Introduction (Ln 73).

Confined with ARCHER2: Lines 158-160 suggest a confinement to ARCHER2, which may limit the generalizability of the findings. Authors should clarify whether the method is applicable to other computing platforms and address any potential limitations in this regard.

- Response:** As described in the text, the parallelisation of uDALES is based on 2DECOMP&FFT, which has been used as
- 105 the basis for several open source projects, most notably the open-source DNS framework XCompact3D (Bartholomew et al., 2020), and has been used across all major supercomputing (CPU-based) platforms worldwide. We are currently working on

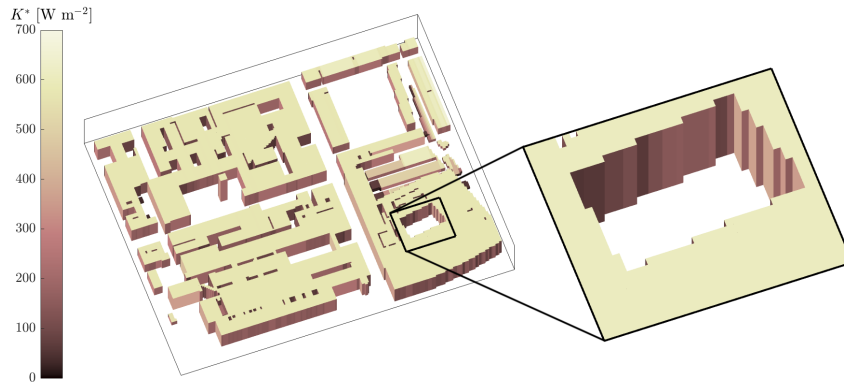


Figure 1. Net shortwave radiation (K^*) on buildings for the demonstration case in Suter et al. (2022). Note that the ground surfaces have been excluded from the visualisation for clarity.

preparing the code for use with GPUs. At the end of Sect. 3.1 we have added: "2DECOMP&FFT has been developed for cross-platform usage and has been tested on all major supercomputer architectures (Li and Laizet, 2010; Rolfo et al., 2023), ensuring excellent portability of uDALES."

110 **Figure 14:** The presence of incoming longwave radiation in Figure 14 should be clearly indicated or discussed in the caption to provide a comprehensive understanding of the depicted variables.

Response: We have changed Ln 496 onwards to: "... the leeward and side faces have reduced incoming longwave radiation for the same reasons given for the shortwave. This is consistent with the fact that the net longwave in Fig. 14 is less negative, and the outgoing longwave is directly determined by surface temperature, which is lower in the v1 rotated case. The temperature of the leeward face is lower because it has less available energy due to the reduced shortwave, which also acts to reduce the sensible heat and conductive fluxes...".

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References

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- 120 Grylls, T. and van Reeuwijk, M.: Tree model with drag, transpiration, shading and deposition: Identification of cooling regimes and large-eddy simulation, *Agricultural and Forest Meteorology*, 298, 108 288, 2021.
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